DAta Mining & Exploration Program

Dipartimento di Scienze Fisiche
Università di Napoli "Federico II"

ISTITUTO NAZIONALE di ASTROFISICA
OSSERVATORIO ASTRONOMICO di CAPODIMONTE

CALTECH

DAME Suite α-release

User's Guide

DAME-MAN-NA-0007

Issue: 1.1
Date: June 28, 2010
Author: M. Brescia

Doc. : AlphaReleaseUserGuide_DAME-MAN-NA-0007-Rel1.1

INAF-OACN

IVOA

This document contains proprietary information of DAME project Board. All Rights Reserved.

DAta Mining & Exploration Program

"Quelli che s'innamoran di pratica sanza scienza, son come 'l nocchiere, ch'entra in navilio sanza timone o bussola, che mai ha certezza di dove si vada"
Leonardo Da Vinci

"No great pyramid was built in a day nor shall be any great software without documentation"
Linus Torvald

"The future of Science is e-Science. e-Science is where Information Technology meets scientists"
Jim Gray

"Artificial Intelligence is the exciting new effort to make computers think . . . machines with minds, in the full and literal sense"
John Haugeland

"*Always two there are… a master and an apprendist… …the Force runs strong in your family!...*"
Yoda, Jedi master

DAME Program
"we make science discovery happen"

This document contains proprietary information of DAME project Board. All Rights Reserved.

INDEX

1 Purpose 6
2 Introduction 7
3 Machine Learning Theoretical Overview 8
3.1 Supervised Machine Learning 9
3.2 The functionality domains 10
3.2.1 Classification 10
3.2.1.1 Confusion Matrix 11
3.2.1.2 K-fold Cross Validation 12
3.2.2 Regression 13
3.3 The Machine Learning Models 15
3.3.1 Multi Layer Perceptron 15
3.3.1.1 Learning by Back Propagation 18
3.3.1.2 Generalization and statistics 20
3.3.1.2.1 Cross Entropy 21
3.3.1.3 MLP Practical Rules 23
3.3.1.3.1 Selection of neuron activation function 24
3.3.1.3.2 Scaling input and target values 24
3.3.1.3.3 Number of hidden nodes 25
3.3.1.3.4 Number of hidden layers 25
3.3.1.3.5 Initializing Weights 25
3.3.1.3.6 Momentum 25
3.3.1.3.7 Learning rate 26
3.3.1.4 Implementation Details 26
4 The Data Mining Suite User's Manual 29
4.1 Overview 30
4.2 User Registration and Access 31
4.3 The command icons 32
4.4 Workspace Management 33
4.5 Header Area 37
4.6 Data Management 38
4.6.1 Upload user data 38
4.6.2 Create dataset files 40
4.6.2.1 Feature Selection 41
4.6.2.2 Column Ordering 42
4.6.2.3 Sort Rows by Column 44
4.6.2.4 Column Shuffle 45
4.6.2.5 Row Shuffle 46
4.6.2.6 Split by Rows 47
4.6.2.7 Dataset Scale 48
4.6.2.8 Single Column Scale 49
4.6.3 Download data 51
4.6.4 Moving data files 51
4.7 Experiment Management 52
4.7.1 Re-use of already trained networks 56
5 A practical example 60
5.1.1 The scientific problem: Photometric redshifts estimation 60
5.1.2 The Base of Knowledge (BoK) 61
5.1.3 Dataset Manipulation 62
5.1.4 Experiment execution 62
5.1.5 Experiment Results 64

This document contains proprietary information of DAME project Board. All Rights Reserved.

TABLE INDEX

Tab. 1 – The DM models available in DAME alpha release 30
Tab. 2 – Header Area Menu Options 37
Tab. 3 – Abbreviations and acronyms 68
Tab. 4 – Reference Documents 69
Tab. 5 – Applicable Documents 70

FIGURE INDEX

Fig. 1 – Where AI may fit into a knowledge process 8
Fig. 2 – A workflow based on supervised learning models 9
Fig. 3 – An example of confusion matrix for a 3-class classification problem 12
Fig. 4 – Some cases of K-fold cross validation 12
Fig. 5 – leave-one-out cross validation 13
Fig. 6 – Example of a SLP to calculate the logic AND operation 17
Fig. 7 – A MLP able to calculate the logic XOR operation 17
Fig. 8 – A MLP network trained by Back Propagation rule 19
Fig. 9 – The sigmoid function and its first derivative 24
Fig. 10 – Typical Layered Application Architecture 29
Fig. 11 – Suite functional hierarchy 30
Fig. 12 – The user login form to access at the web application 32
Fig. 13 – The Web Application starting page (home) 32
Fig. 14 – The Web Application main commands 33
Fig. 15 – The right sequence to configure and execute an experiment workflow 34
Fig. 16 – the button "New Workspace" at left corner of workspace manager window 34
Fig. 17 – the form field that appears after pressing the "New Workspace" button 35
Fig. 18 – the active workspace created in the Workspace List Area 35
Fig. 19 – The GUI Header Area with all submenus open 37
Fig. 20 – The Upload data feature open in a new tab 38
Fig. 21 – The Upload data from external URI feature 39
Fig. 22 – The Upload data from Hard Disk feature 39
Fig. 23 – The Uploaded data (train.fits) in the Files Manager sub window 40
Fig. 24 – The dataset editor tab with the list of available operations 41
Fig. 25 – The Feature Selection operation – step 1 41
Fig. 26 – The Feature Selection operation – step 2 42
Fig. 27 – The Feature Selection operation – the new file created 42
Fig. 28 – The Column Ordering operation – step 1 43
Fig. 29 – The Column Ordering operation – step 2 43
Fig. 30 – The Column Ordering operation – the new file created 43
Fig. 31 – The Sort Rows by Column operation – step 1 44
Fig. 32 – The Sort Rows by Column operation – step 2 44
Fig. 33 – The Sort Rows by Column operation – the new file created 45
Fig. 34 – The Column Shuffle operation – step 1 45
Fig. 35 – The Column Shuffle operation – the new file created 46
Fig. 36 – The Row Shuffle operation – step 1 46
Fig. 37 – The Row Shuffle operation – the new file created 47
Fig. 38 – The Split by Rows operation – step 1 47
Fig. 39 – The Split by Rows operation – step 2 48

This document contains proprietary information of DAME project Board. All Rights Reserved.

Fig. 40 – The Split by Rows operation – the new files created *48*
Fig. 41 – The Dataset Scale operation – step 1 ..... *49*
Fig. 42 – The Dataset Scale operation – the new file created *49*
Fig. 43 – The Single Column Scale operation – step 1 ..... *50*
Fig. 44 – The Single Column Scale operation – step 2 ..... *50*
Fig. 45 – The Single Column Scale operation – the new file created *51*
Fig. 46 – Creating a new experiment (by selecting icon "Experiment" in the workspace) *52*
Fig. 47 – The new tab reporting the list of functionality-model couples available for experiments *53*
Fig. 48 – The use case selection for the experiment *53*
Fig. 49 – The experiment parameter list for the use case "Full" in the regression case *54*
Fig. 50 – The experiment parameter list for the use case "Full" in the classification case *54*
Fig. 51 – The experiment parameter list for the use case "Train" *55*
Fig. 52 – The experiment parameter list for the use case "Test" *55*
Fig. 53 – The experiment parameter list for the use case "Run" *56*
Fig. 54 – Some different state of two concurrent experiments *56*
Fig. 55 – The operation to "move" an output file in the Workspace input file list *57*
Fig. 56 – The choice of input parameters of Run use case experiment *58*
Fig. 57 – Some different state of two concurrent experiments *59*
Fig. 58 – The relation between redshift, color and source observed fluxes *60*
Fig. 59 – The 5 columns and first 13 rows of train.dat input file *61*
Fig. 60 – The complete flow-chart of the experiment with MLP model *62*
Fig. 61 – The selection of train.fits as Train Set *63*
Fig. 62 – The selection of train.fits as Test Set and all fields compiled *63*
Fig. 63 – The myFirstExp output file list after the end of experiment *65*
Fig. 64 – The contents of Full.log *65*
Fig. 65 – The contents of Full.tra (left) and Full.tes (right) *66*
Fig. 66 – The contents of Full.csv *66*
Fig. 67 – The contents of Full.tes.jpeg *66*
Fig. 68 – The contents of Full.csv.jpeg *67*
Fig. 69 – Best Trend of zspec versus zphot redshifts for the Main Galaxy sample *67*

This document contains proprietary information of DAME project Board. All Rights Reserved.

1 Purpose

The present document has been extracted from the DAME Book[1], a big document containing all scientific and technological information behind the strategy of DAME, including design, development and implementation issues, together with instruction on how to use and maintain the entire infrastructure.

This document is the reference manual of the official alpha release of the data mining Suite. The alpha is available for test at the following address: http://143.225.93.239:8080/MyDameFE/

So far it has the basic role to support testing users (the victims…!) to use the software toolset in the right and more satisfying way.

The available features, in terms of data mining models and functional use cases for scientific experiments, are voluntarily limited within the alpha release, although sufficient to verify the internal mechanisms and user-machine interaction modes at the base of the DM Suite and of its next releases.
As the reader probably already knows, the data mining models provided in DAME are derived from the machine learning and Artificial Intelligence paradigms. Some of the end users in principle could not be familiar with such models. So far, a theoretical quick and practice-oriented overview of such techniques is required.
The document is hence organized as follows:

- Chapter 2 is a simple Introduction to DAME Program "proposition value";
- Chapter 3 introduces the reader through theoretical and algorithmic aspects concerning machine learning models and functional domains currently available in the released software;
- Chapter 4 is the user's reference and guide to use the DM Suite current release;
- Chapter 5 reports a practical example of scientific use case solved by the DM Suite current release;
- Last pages host tables with "Abbreviations & Acronyms", "Reference" and "Applicable" document lists and the acknowledgments. All over the document the references are labeled as [Rxx] for "Reference" documents and [Axx] for "Applicable" documents (xx is the incremental index as reported in the list tables). "Applicable" documents are not public references (technical documents internal to the DAME working group) included for quick technical references. Users external to the working group may ask to consult (privately) these documents by e-mail, motivating the reasons. The complete list of the internal documentation is available at the following address of the program official website: http://voneural.na.infn.it/DAME_DOCUMENTATION_LIST.html

[1] Currently under preparation.

This document contains proprietary information of DAME project Board. All Rights Reserved.

2 Introduction

DAME arises as a single project at the beginning of 2007. The original name was VO-Neural, derived from earlier Astroneural project, whose main goal was to create a software framework to solve specific astrophysical problems by employing experienced methodologies coming from Machine Learning and Artificial Intelligence paradigms and architectures. After first two years of design activity, VO-Neural definitely changes into DAME.
Since the beginning of the project, its members observed the following facts.
The explosion of technology progress in digital processing, computer Science, high performance and distributed computing, astronomical telescopes and focal plane instrumentation, imposed a new approach to make Science, able to explore in an efficient way the incoming "tsunami" of petabytes of data collected in worldwide distributed archives and data centres: the new frontier became the e-Science.
Indeed, this trend has rapidly issued the fourth paradigm of Science, recently recognized at a planetary level, after theory, experimentation and simulations: data mining, or equivalently, Knowledge Discovery in Databases (KDD), [R6].
These considerations convinced our group to pursue their scientific goals from a new, more organized, coherent and efficient perspective. So far, the idea was to create a program, as a whole infrastructure capable to merge in an homogeneous way scientific products with the state of the art of technology and astrophysics trends, where the multi-disciplinary experience and the data mining research would be the engine of the common goal. Moreover, the immediate consequence was the awareness that such an infrastructure could represent a standard gateway to accomplish the fourth paradigm for further discoveries in the e-Science, in particular e-Astrophysics, [A1]. In other words, a product to be shared with the entire scientific community in an "*open and easy way*".
Open means basically easily extendable in terms of functionalities and data mining models able to be employed in the general astrophysics research and data exploration at large.
While the term *easy* is referred to the features offered to the community users, in terms of high computing power and user-friendly scientific applications available "at one click", through a simple web browser.
In other words, this product inherits advanced technological aspects made available to users in an absolutely transparent way, leaving them to focus their brain energies to organize and execute scientific experiments and workflows[2].

The only effort required to the end user is to have a bit of faith in Artificial Intelligence and a little amount of patience to learn basic principles of its models and strategies.

By merging for fun two famous commercial taglines we say: "*Think different, Just do it!*"
(casually this is an example of *text mining*...!)

[2] Workflow is hereinafter synonymous of pipeline.

This document contains proprietary information of DAME project Board. All Rights Reserved.

3 Machine Learning Theoretical Overview

One of main breakthroughs in modern Astrophysics is the reached physical limit of observations (single photon counting) at almost all wavelengths, with giant and by now linear detectors. So far, like all scientific disciplines focusing their discoveries on collected data exploration, there is a strong need to employ e-science methodology and tools in order to gain new insights on the Universe. But this mainly depend on the capability to recognize patterns or trends in the parameter space (i.e. physical laws), possibly by overcoming the human limit of 3D brain vision, and to use known patterns (coming from observations and simulations as well) as BoK (Base of Knowledge) to infer knowledge on self-adaptive models in order to make them able to generalize feature correlations and to gain new discoveries (for example outliers identification) through the unbiased exploration of new collected data. These requirements are perfectly matching the paradigm of machine learning techniques based on the Artificial Intelligence postulate, [R7].

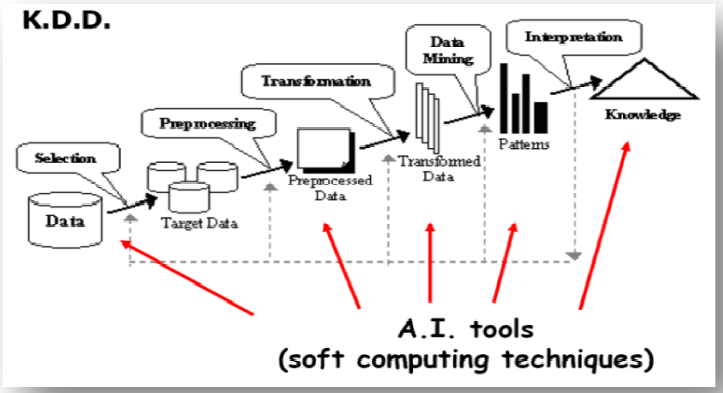


Fig. 1 – Where AI may fit into a knowledge process

Hence, as shown in Fig. 1, at all steps of a scientific pipeline process, machine learning rules can be applied, [R8]. Let us better know this methodology. It exists a basic dichotomy in Machine Learning, [R2, R3], by distinguish between supervised and unsupervised methodologies, as described in the following.
The Greek philosopher Aristotle was one of the first to attempt to codify "right thinking," that syllogism is, irrefutable reasoning processes. His syllogisms provided patterns for argument structures that always yielded correct conclusions when given correct premises; for example, "Socrates is a man; all men are mortal; therefore, Socrates is mortal." These laws of thought were logic supposed to govern the operation of the mind; their study initiated the field called “logic”**.**
Logicians in the 19th century developed a precise notation for statements about all kinds of things in the world and about the relations among them[3].
By 1965, programs existed that could, in principle, solve *any* solvable problem described in logicist logical notation. The so-called logicist tradition within Artificial Intelligence hopes to build on such programs to create intelligent systems and the Machine Learning theory represents their demonstration discipline. A reinforcement in this direction came out by integrating Machine Learning paradigm with statistical principles following the Darwin’s Nature evolution laws, [R1, R11].

[3] Contrast this with ordinary arithmetic notation, which provides mainly for equality and inequality statements about numbers.

This document contains proprietary information of DAME project Board. All Rights Reserved.

3.1 Supervised Machine Learning

In supervised machine learning we have a set of data points or *observations* for which we know the desired output, class, *target variable* or *outcome*. The outcome may take one of many values called *classes* or *labels*. A classic example is that given a few thousand emails for which we know whether they are spam or ham (their labels), the idea is to create a model that is able to deduce whether new, unseen emails are spam or not. In other words, we are creating a mapping function where the inputs are the email's sender, subject, date, time, body, attachments and other attributes, and the output is a prediction as to whether the email is spam or ham. The *target variable* is in fact providing some level of *supervision* in that it is used by the learning algorithm to adjust parameters or make decisions that will allow it to predict labels for new data. Finally of note, when the algorithm is predicting labels of observations we call it a *classifier*. Some classifiers are also capable of providing a probability of a data point belonging to class in which case it is often referred to a probabilistic model or a regression - not to be confused with a statistical regression model.
A common workflow approach for supervised learning analysis is shown in the diagram below (Fig. 2).

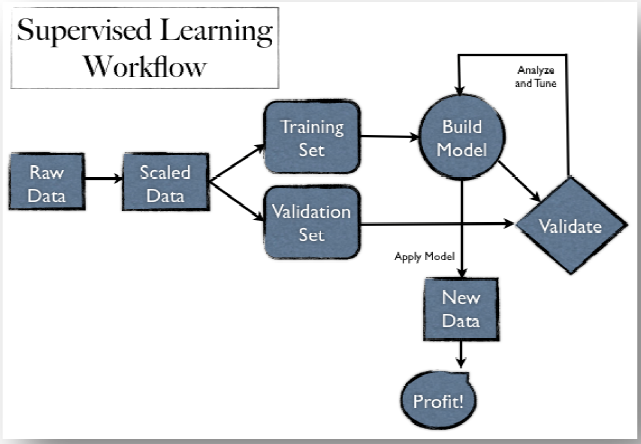


Fig. 2 – A workflow based on supervised learning models

The process is:

1. *Scale and prepare training data*: First we build input vectors that are appropriate for feeding into our supervised learning algorithm.
2. *Create a training set and a validation set* by randomly splitting the universe of data. The training set is the data that the classifier uses to learn how to classify the data, whereas the validation set is used to feed the already trained model in order to get an error rate (or other measures and techniques) that can help us identify the classifier's performance and accuracy. Typically you will use more training data (maybe 80% of the entire universe) than validation data. Note that there is also cross-validation), but that is beyond the scope of this article.
3. *Train the model*. We take the training data and we feed it into the algorithm. The end result is a model that has learned (hopefully) how to predict our outcome given new unknown data.
4. *Validation and tuning*: After we've created a model, we want to test its accuracy. It is critical to do this on data that the model has not seen yet - otherwise you are cheating. This is why on step 2 we separated out a subset of the data that was not used for training. We are indeed testing our model's generalization capabilities. It is very easy to learn every single combination of input vectors and their mappings to the output as observed on the training data, and we can achieve a very low error in

This document contains proprietary information of DAME project Board. All Rights Reserved.

doing that, but how does the very same rules or mappings perform on new data that may have different input to output mappings? If the classification error of the validation set is very big compared to the training set's, then we have to go back and adjust model parameters. The model will have essentially memorized the answers seen in the training data, losing its generalization capabilities. This is called over fitting, and there are various techniques for overcoming it.

5. Validate the model's performance. There are numerous techniques. The model's accuracy can be improved by changing its structure or the underlying training data. If the model's performance is not satisfactory, change model parameters, inputs and or scaling, go to step 3 and try again.
6. Use the model to classify new data. In production. Profit!

3.2 The functionality domains

In the data mining scenario, the machine learning model choice should always be accompanied by the functionality domain. To be more precise, some machine learning models can be used in a same functionality domain, because it represents the functional context in which it is performed the exploration of data.
Examples of such domains are:

- Dimensional reduction;
- Classification;
- Regression;
- Clustering;
- Segmentation;
- Statistical data analysis;
- Forecasting;
- Data Mining Model Filtering;

In the following we focus the attention on Classification and Regression only, being the two functional domains available in the current alpha release of the data mining application Suite.

3.2.1 Classification

Statistical classification is a procedure in which individual items are placed into groups based on quantitative information on one or more features inherent to the items (referred to as features) and based on a training set of previously labelled items.
A classifier is a system that performs a mapping from a feature space X to a set of labels Y. Basically a classifier assigns a pre-defined class label to a sample.
Formally, the problem can be stated as follows: given training data {(x_1,y_1),...,(x_n, y_n)} (where x_i are vectors) a classifier h:X->Y maps an object x ε X to its classification label y ε Y.

Different classification problems could arise:

a) crispy classification: given an input pattern x (vector) the classifier returns its computed label y (scalar).

b) probabilistic classification: given an input pattern x (vector) the classifier returns a vector y which contains the probability of y_i to be the "right" label for x. In other words in this case we seek, for each input vector, the probability of its membership to the class y_i (for each y_i).

This document contains proprietary information of DAME project Board. All Rights Reserved.

Both cases may be applied to both "two-class" and "multi-class" classification. So the classification task involves, at least, three steps:

- *training*, by means of a training set (INPUT: patterns and target vectors, or labels; OUTPUT: an evaluation system of some sort);
- *testing*, by means of a test set (INPUT: patterns and target vectors, requiring a valid evaluation system from point 1; OUTPUT: some statistics about the test, confusion matrix, overall error, bitfail error, as well as the evaluated labels);
- *evaluation*, by means of an unlabelled dataset (INPUT: patterns, requiring a valid evaluation systems; OUTPUT: the labels evaluated for each input pattern);

Because of the supervised nature of the classification task, the system performance can be measured by means of a test set during the testing procedure, in which unseen data are given to the system to be labelled.
The overall error somehow integrates information about the classification goodness. However, when a data set is unbalanced (when the number of samples in different classes varies greatly) the error rate of a classifier is not representative of the true performance of the classifier. A confusion matrix can be calculated to easily visualize the classification performance: each column of the matrix represents the instances in a predicted class, while each row represents the instances in an actual class. One benefit of a confusion matrix is the simple way to see if the system is mixing two classes.
Optionally (some classification methods does not require it by its nature or simply as a user choice), one could need a validation procedure.
Validation is the process of checking if the classifier meets some criterion of generality when dealing with unseen data. It can be used to avoid over-fitting or to stop the training on the base of an "objective" criterion.
With “objective” we intend a criterion which is not based on the same data we have used for the training procedure. If the system does not meet this criterion it can be changed and then validated again, until the criterion is matched or a certain condition is reached (for example, the maximum number of epochs). There are different validation procedures. One can use an entire dataset for validation purposes (thus called validation set); this dataset can be prepared by the user directly or in an automatic fashion.
In some cases (e.g. when the training set is limited) one could want to apply a "cross validation" procedure, which means partitioning a sample of data into subsets such that the analysis is initially performed on a single subset, while the other subset(s) are retained for subsequent use in confirming and validating the initial analysis.
Different types of cross validation may be implemented, e.g. k-fold, leave-one-out, etc.
Summarizing we can safely state that a common classification training task involves:

- the training set to compute the model;
- the validation set to choose the best parameters of this model (in case there are "additional" parameters that cannot be computed based on training);
- the test data as the final "judge", to get an estimate of the quality on new data that are used neither to train the model, nor to determine its underlying parameters or structure or complexity of this model;

The validation set may be provided by the user, extracted from the software or generated dynamically in a cross validation procedure. In the following we underline some practical aspects connected with the validation techniques, as implemented in our classification models.

3.2.1.1 Confusion Matrix

This is a simple diagnostic instrument useful to estimate the efficiency of the classification model (such as a supervised neural network). It basically consists in a matrix with the values of target vector and the output values produced from the model, respectively, on its rows and columns, [A12]. In addition it allows to

This document contains proprietary information of DAME project Board. All Rights Reserved.

calculate the success rate, e.g. the percentage of objects correctly classified from the model. The number of "bit fault" that the model badly classifies and the percentage of correctly classified objects for each class.
In the matrix the element corresponding to row i and column j is the absolute number or case percentage of "true" class i classified in the class j. On the main diagonal the correct classified cases are reported. The others are classification errors.

	A	B	C	Totale	
A	60	14	13	87	69,0%
B	15	34	11	60	56,7%
C	11	0	42	53	79,2%
Totale	86	48	66	200	68,0%

Fig. 3 – An example of confusion matrix for a 3-class classification problem

In the example of Fig. 3 we have a 3-class classification problem results. The original training set consists of 200 patterns.
In the class A there are 87 cases: 60 correctly classified as A; 27 wrongly classified, of which 14 as B and 13 as C.
So far, for the class A the accuracy is 60 / 87 = 69,0%. For the class B the accuracy is 34 / 60 = 56,7% and for class C 42 / 53 = 79,2%.
The whole accuracy is hence: (60 + 34 + 42) / 200 = 136 / 200 = 68,0%. The errors (bad classification) are then 32%, e.g. 64 cases on 200 patterns.

The classification result depends not only on the percentages, but also on the relevance of single kinds of errors. In the example, if class C is the most important to be classified, the final result of the classification can be considered successful.

3.2.1.2 K-fold Cross Validation

The cross validation is a statistical method useful to validate a predictive classification model. Having a data sample this is divided into subsets, some of them used for the training phase (training set), while the others employed to compare the model prediction capability (validation set). By varying the value of K (different splitting of the data sets) it is possible to evaluate the prediction accuracy of the trained model, Fig. 4.

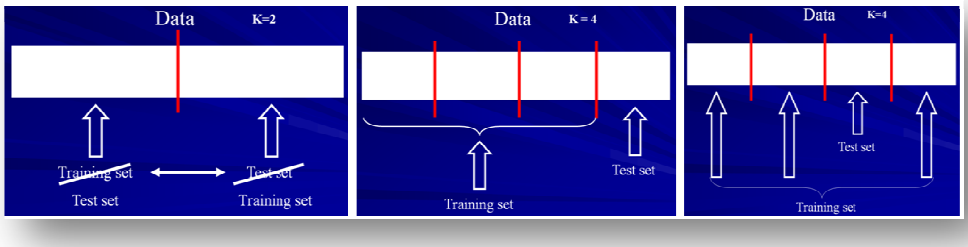


Fig. 4 – Some cases of K-fold cross validation

The **K-fold cross-validation** divides the whole dataset into K subsets, each of them is alternately excluded from the validation set.

This document contains proprietary information of DAME project Board. All Rights Reserved.

There is also a special case, named l**eave-one-out cross validation,** where alternately only one pattern is excluded at each validation run, Fig. 5.

Fig. 5 – leave-one-out cross validation

In practice all data are used for the training and test phases in an independent way. In this case we obtain K classifiers ($2 \leq K \leq n$) whose outputs can be used to obtain a mean evaluation. The downside of this method is that it could result very expensive in terms of computing time in case of massive datasets.

3.2.2 Regression

Regression methods bring out relations between variables, especially whose relation is imperfect (i.e it has not one y for each given x). Just as an example, the relation in a DM design team between brain weight and working capability of the members is a typical "imperfect relationship" (any reference is purely casual…).
The term *regression* is historically coming from biology in genetic transmission through generations, where for example it is known that tall fathers have tall sons, but not as tall on the average as the fathers. The trend to transmit on average genetic features, but not exactly in the same quantity, was what the scientist Galton defined as *regression*, more exactly *regression toward the mean*.
This is the first item I founded through a short immersion on the argument.

But what is regression? Strictly speaking it is very difficult to find a precise definition. We prefer to deal with two meanings for regression, that can be addressed as *data table statistical correlation* (usually column averages) and as *fitting of a function*.

About the first meaning, let start with a very generic example: suppose to have two variables x and y, where for each small interval of x there is a distribution of corresponding y. We can always compute a summary of the y values for that interval. The summary might be for example the mean, median or even the geometric mean. Let fix the points $(x_i, \overline{y_i})$, where x_i is the center of the ith interval and $\overline{y_i}$ the average y for that interval. Then the fixed points will fall close to a curve that could summarize them, possibly close to a straight line. Such a smooth curve approximates the regression curve called the *regression of y on x*. By generalizing the example, the typical application is when the user has a table (let say a series of input patterns coming from any experience or observation) with some correspondences between intervals of x (table raws) and some distributions of y (table columns), representing a generic correlation not well known (i.e. imperfect as introduced above) between them. Once we have such a table, we want for example to clarify or accent the relation between the specific values of one variable and the corresponding values of the other. If we want an average, we might compute the mean or median for each column. Then to get a regression, we might plot these averages against the midpoints of the class intervals.
Given the example in mind let's try to extrapolate the formal definition of regression (in its first meaning).
In a mathematical sense, when for each value of x there is a distribution of y, with density f(y|x) and the mean[4] value of y for that x given by

$$\overline{y}(x) = \int_{-\infty}^{+\infty} y f(y \mid x) dy$$

[4] Here the use of the mean as statistical operator is only an example. It can be replaced by the median or other more complex methods.

This document contains proprietary information of DAME project Board. All Rights Reserved.

then the function defined by the set of ordered pairs $((x, \bar{y}(x))$ is called the regression of y on x. Depending on the statistical operator used, the resulting regression line or curve on the same data can present a slightly different slope.
In the practical astrophysical cases, we usually do not have continuous populations with known functional forms. But the data may be very extensive. In these cases it is possible to break one of the variables into small intervals and compute averages for each of them. Then, without severe assumptions about the shape of the curve, essentially get a regression curve. What the regression curve does is essentially to give a, let say, "big summary" for the averages for the distributions corresponding to the set of x's. One can go further and compute several different regression curves corresponding to the various percentage points of the distributions and thus get a more complete picture of the input data set. Of course often it is an incomplete picture for a set of distributions! But in this first meaning of regression, when the data are more sparse, we may find that sampling variation makes impractical to get a reliable regression curve in the simple averaging way described. From this assumption, it descends the second meaning of regression.
Usually it is possible to introduce a smoothing procedure, applying it either to the column summaries or to the original values of y's (of course after an ordering of y values in terms of increasing x). In other words we assume a shape for the curve describing the data, for example linear, quadratic, logarithmic or whatever. Then we fit the curve by some statistical method, often least-squares. In practice, we do not pretend that the resulting curve has the perfect shape of the regression curve that would arise if we had unlimited data, but simply we obtain an approximation. In other words we intend the regression of data in terms of *forced fitting of a functional form*. The real data present intrinsic conditions that make this second meaning as the official regression use case, instead of the first, i.e. *curve connecting averages of column distributions*. We ordinarily choose for the curve a form with relatively few parameters and then we have to choose the method to fit it. In many manuals sometimes it might be founded a definition probably not formally perfect, but very clear: *by regressing one y variable against one x variable means to find a* ***carrier*** *for x*.
This introduce possible more complicated scenarios in which more than one carrier of data can be founded. In these cases it has the advantage that the geometry can be kept to three dimensions (with two carriers) up to n-dimensional spaces (n>3, with more than two carriers regressing input data). Clearly, both choosing the set of carriers from which a final subset is to be drawn and choosing that subset can be most disconcerting processes.
In substance we can declare a simple, important use of regression, consisting in:
To get a summary of data, i.e. to locate a representative functional operator of the data set, in a statistical sense (first meaning) or via an approximated trend curve estimation (second meaning).
And a more common use of regression:

- For evaluation of unknown features hidden into the data set;
- For prediction, as when we use information from several weather or astronomical seeing stations to predict the probability of rain or the turbulence growing in the atmosphere;
- For exclusion. Usually we may know that x affects y, and one could be curious to know whether z affects[5] y too. In this case one approach would take the effects of x out of y and see if what remains is associated with z. In practice this can be done by an iterative fitting procedure by evaluating at each step the residual of previous fitting.

This is not exhaustive of the regression argument, but simple considerations to help the understanding of the regression term and the possibility to extract basic specifications for the use case characterization in the design phase.

[5] Here "affects" is a shorthand for "is associated with, possibly, but not certainly, through a causal mechanism".

This document contains proprietary information of DAME project Board. All Rights Reserved.

3.3 The Machine Learning Models

This paragraph is intended to furnish a theoretical overview of some machine learning models to be associated with single or multiple functionality domains, in order to be used to perform practical scientific experiments with such techniques. Only models foreseen to be implemented in the DAME infrastructure will be treated.

3.3.1 Multi Layer Perceptron

The MLP architecture is one of the most typical *feed-forward* neural network model, [R9]. The term feed-forward is used to identify basic behavior of such neural models, in which the impulse is propagated always in the same direction, e.g. from neuron input layer towards output layer, through one or more hidden layers (the network brain), by combining weighted sum of *weights associated to all neurons* (except the input layer).
As easy to understand, the neurons are organized in layers, with proper own role. The input signal, simply propagated throughout the neurons of the input layer, is used to stimulate next hidden and output neuron layers. The output of each neuron is obtained by means of an *activation function*, applied to the weighted sum of its inputs. Different shape of this activation function can be applied, from the simplest *linear* one up to *sigmoid*, *arctan* or *tanh* (or a customized function ad hoc for the specific application). The number of hidden layers represents the degree of the complexity achieved for the energy solution space in which the network output moves looking for the best solution. As an example, in a typical classification problem, the number of hidden layers indicates the number of hyper-planes used to split the parameter space (i.e. number of possible classes) in order to classify each input pattern.

There is a special type of activation function, called ***softmax***, [A13].
As known the activation function can be either linear or non-linear, depending on whether the network must learn a regression problem or should perform a classification.
Activation functions, for the hidden units, introduce the non linearity into the network. Without non linearity, the hidden units would not render the NN more powerful than just the perceptrons with only input and output units (the linear function of linear functions is again a linear function). In other words, it is the non linearity (i.e., the capability to represent non linear functions) that makes multilayer networks so powerful.
For the hidden units, sigmoid activation functions (for binary problems), see equation (2), or softmax (for multi class problem), are usually better to use instead of the threshold activation functions, see equation (1).

$$f(x) = \begin{cases} 0 \text{ if } a < 0 \\ 1 \text{ else} \end{cases} \qquad (1)$$

$$f(x) = \frac{1}{1+e^{-a}} \qquad (2)$$

Networks with threshold units are difficult to train, because the error function is stepwise constant, hence the gradient either does not exist or is zero, thus making it impossible to use back propagation (a powerful and computationally efficient algorithm for finding the derivatives of an error function with respect to the weights and biases in the network) or the more efficient gradient-based training methods.
With sigmoid units, a small change in the weights will usually produce a large change in the outputs, which makes it possible to tell whether that change in the weights is good or useless. With threshold units, a small change in the weights will often produce no change in the outputs. For the output units, activation functions suited to the distribution of the target values are:

This document contains proprietary information of DAME project Board. All Rights Reserved.

- For binary (0/1) targets, the logistic sigmoid function is an excellent choice;
- For categorical targets using 1-of-C coding, the softmax activation function is the natural extension of the logistic function;
- For continuous-valued targets with a bounded range, the logistic and hyperbolic tangent functions can be used, where you either scale the outputs to the range of the targets or scale the targets to the range of the output activation function ("scaling" means multiplying by and adding appropriate constants);
- If the target values are positive but have no known upper bound, you can use an exponential output activation function, but you must beware of overflow;
- For continuous-valued targets with no bounds, use the identity or "linear" activation function (which amounts to no activation function) unless you have a very good reason to do otherwise.

There are certain natural associations between output activation functions and various noise distributions. The output activation function is the inverse of what statisticians call the "link function".

In order to ensure that the outputs can be interpreted as posterior probabilities, they must be comprised between zero and one, and their sum must be equal to one. This constraint also ensures that the distribution is correctly normalized. In practice this is, for multi-class problems, achieved by using a softmax activation function in the output layer. The purpose of the softmax activation function is to enforce these constraints on the outputs. Let the network input to each output unit be q_i, i = 1,...,*c*, where *c* is the number of categories. Then the softmax output p_i is:

$$p_i = \frac{e^{q_i}}{\sum_{j=1}^{c} e^{q_j}}$$

Statisticians usually call softmax a "multiple logistic" function. Softmax equation is also known as normalized exponential function. It reduces to the simple logistic function when there are only two categories. Suppose you choose to set $q_2 = 0$:

$$p_1 = \frac{e^{q_1}}{\sum_{j=1}^{c} e^{q_j}} = \frac{e^{q_1}}{e^{q_1} - e^{0}} = \frac{1}{1+e^{-q_1}}$$

The term softmax is used because this activation function represents a smooth version of the winner-takes-all activation model in which the unit with the largest input has output +1 while all other units have output 0.

The base of the MLP is the **Perceptron,** a type of artificial neural network invented in 1957 at the Cornell Aeronautical Laboratory by Frank Rosenblatt. It can be seen as the simplest kind of feedforward neural network: a linear classifier. The Perceptron is a binary classifier which maps its input *x* (a real-valued vector) to an output value *f*(*x*) (a single binary value) across the matrix.

$$f(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{w} \cdot \boldsymbol{x} + b > 0 \\ 0 & \text{else} \end{cases}$$

where *w* is a vector of real-valued weights and $\boldsymbol{w} \cdot \boldsymbol{x}$ is the dot product (which computes a weighted sum). *b* is the 'bias', a constant term that does not depend on any input value. The value of *f*(*x*) (0 or 1) is used to classify *x* as either a positive or a negative instance, in the case of a binary classification problem.

This document contains proprietary information of DAME project Board. All Rights Reserved.

If *b* is negative, then the weighted combination of inputs must produce a positive value greater than | *b* | in order to push the classifier neuron over the 0 threshold. Spatially, the bias alters the position (though not the orientation) of the decision boundary. The Perceptron learning algorithm does not terminate if the learning set is not linearly separable. The Perceptron is considered the simplest kind of feed-forward neural network.
The earliest kind of neural network is a S*ingle Layer Perceptron* (SLP) network, which consists of a single layer of output nodes; the inputs are fed directly to the outputs via a series of weights. In this way it can be considered the simplest kind of feed-forward network. The sum of the products of the weights and the inputs is calculated in each node, and if the value is above some threshold (typically 0) the neuron fires and takes the activated value (typically 1); otherwise it takes the deactivated value (typically -1).

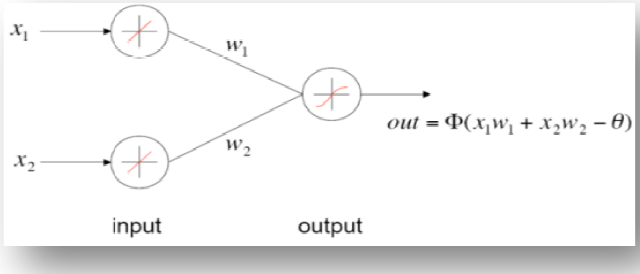


Fig. 6 – Example of a SLP to calculate the logic AND operation

Neurons with this kind of activation function are also called a*rtificial neurons* or *linear threshold units*, as described by Warren McCulloch and Walter Pitts in the 1940s.
A Perceptron can be created using any values for the activated and deactivated states as long as the threshold value lies between the two. Most perceptrons have outputs of 1 or -1 with a threshold of 0 and there is some evidence that such networks can be trained more quickly than networks created from nodes with different activation and deactivation values. SLPs are only capable of learning linearly separable patterns. In 1969 in a famous monograph entitled *Perceptrons* Marvin Minsky and Seymour Papert showed that it was impossible for a single-layer Perceptron network to learn an XOR function.
Although a single threshold unit is quite limited in its computational power, it has been shown that networks of parallel threshold units can approximate any continuous function from a compact interval of the real numbers into the interval [-1,1]. So far, it was introduced the model Multi Layer Perceptron.

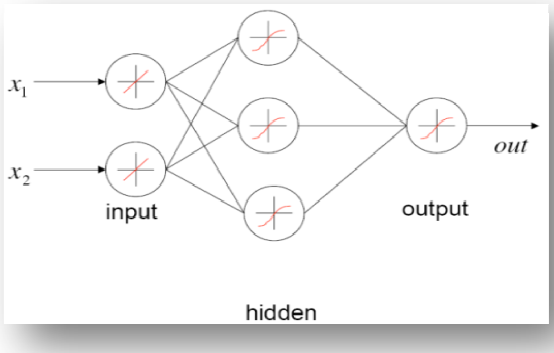


Fig. 7 – A MLP able to calculate the logic XOR operation

This class of networks consists of multiple layers of computational units, usually interconnected in a feed-forward way. Each neuron in one layer has directed connections to the neurons of the subsequent layer. In many applications the units of these networks apply a continuous activation function.

This document contains proprietary information of DAME project Board. All Rights Reserved.

The *universal approximation theorem* [R12] for neural networks states that every continuous function that maps intervals of real numbers to some output interval of real numbers can be approximated arbitrarily closely by a multi-layer Perceptron with just one hidden layer. This result holds only for restricted classes of activation functions, e.g. for the sigmoidal functions.
An extension of the universal approximation theorem states that the two layers architecture is capable of universal approximation and a considerable number of papers have appeared in the literature discussing this property. An important corollary of these results is that, in the context of a classification problem, networks with sigmoidal non-linearity and two layer of weights can approximate any decision boundary to arbitrary accuracy. Thus, such networks also provide universal non-linear discriminate functions. More generally, the capability of such networks to approximate general smooth functions allows them to model posterior probabilities of class membership. Since two layers of weights suffice to implement any arbitrary function, one would need special problem conditions, or requirements to recommend the use of more than two layers. Furthermore, it is found empirically that networks with multiple hidden layers are more prone to getting caught in undesirable local minima.
Astronomical data do not seem to require such level of complexity and therefore it is enough to use just a double weights layer, i.e. a single hidden layer.
The MLP consists of three or more layers (an input and an output layer with one or more *hidden layers*) of nonlinearly-activating nodes. Each node in one layer connects with a certain weight w_{ij} to every node in the following layer.
What is different in such a neural network architecture is typically the learning algorithm used to train the network. It exists a dichotomy between *supervised* and *unsupervised* learning methods.
As in all supervised models, the network must be firstly trained (*training phase*), in which the input patterns are submitted to the network as couples (input, desired known output). The feed-forward algorithm is then achieved and at the end of the input submission, the network output is compared with the corresponding desired output in order to quantify the learning quote. It is possible to perform the comparison in a *batch* way (after an entire input pattern set submission) or *incremental* (the comparison is done after each input pattern submission) and also the *metric* used for the *distance* measure between desired and obtained outputs, can be chosen accordingly problem specific requirements (usually the Euclidean distance is used).
After each comparison and until a desired error distance is unreached (typically the error tolerance is a pre-calculated value or a constant imposed by the user), the weights of hidden layers must be changed accordingly to a particular law or learning technique.
After the training phase is finished (or arbitrarily stopped), the network should be able not only to recognize correct output for each input already used as training set, but also to achieve a certain degree of *generalization*, i.e. to give correct output for those inputs never used before to train it. The degree of generalization varies, as obvious, depending on how “good” has been the learning phase. This important feature is realized because the network doesn’t associates a single input to the output, but it discovers the relationship present behind their association. After training, such a neural network can be seen as a black box able to perform a particular function (input-output correlation) whose analytical shape is a priori not known. In order to gain the best training, it must be as much homogeneous as possible and able to describe a great variety of samples. Bigger the training set, higher will be the network generalization capability.
Despite of these considerations, it should always taken into account that neural networks application field should be usually referred to problems where it is needed high flexibility (quantitative result) more than high precision (qualitative results).

3.3.1.1 Learning by Back Propagation

Multi-layer networks use a variety of learning techniques, the most popular being *back-propagation* (BP). Here, the output values are compared with the correct answer to compute the value of some predefined error-function. By various techniques, the error is then fed back through the network. Using this information, the algorithm adjusts the weights of each connection in order to reduce the value of the error function by some small amount. After repeating this process for a sufficiently large number of training cycles, the network will

This document contains proprietary information of DAME project Board. All Rights Reserved.

usually converge to some state where the error of the calculations is small. In this case, one would say that the network has *learned* a certain target function. To adjust weights properly, one applies a general method for non-linear optimization that is called gradient descent. For this, the derivative of the error function with respect to the network weights is calculated, and the weights are then changed such that the error decreases (thus going downhill on the surface of the error function). For this reason, back-propagation can only be applied on networks with differentiable activation functions.
In general, the problem of teaching a network to perform well, even on samples that were not used as training samples, is a quite subtle issue that requires additional techniques. This is especially important for cases where only very limited numbers of training samples are available. The danger is that the network overfits the training data and fails to capture the true statistical process generating the data. Computational learning theory is concerned with training classifiers on a limited amount of data. In the context of neural networks a simple heuristic, called early stopping, often ensures that the network will generalize well to examples not in the training set.
Other typical problems of the back-propagation algorithm are the speed of convergence and the possibility of ending up in a local minimum of the error function. Today there are practical solutions that make back-propagation in multi-layer perceptrons the solution of choice for many machine learning tasks.

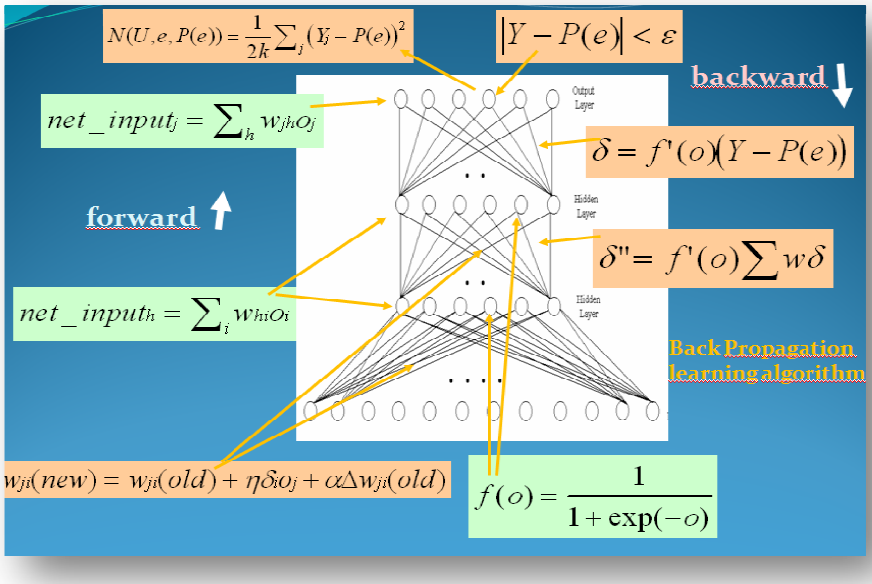

$N(U,e,P(e)) = \frac{1}{2k}\sum_j (Y_j - P(e))^2$
$|Y - P(e)| < \varepsilon$
backward
$net\_input_j = \sum_h w_{jh} o_j$
$\delta = f'(o)(Y - P(e))$
forward
$\delta'' = f'(o)\sum w\delta$
$net\_input_h = \sum_i w_{hi} O_i$
Back Propagation learning algorithm
$w_{ji}(new) = w_{ji}(old) + \eta\delta_i o_j + \alpha\Delta w_{ji}(old)$
$f(o) = \frac{1}{1+\exp(-o)}$

Fig. 8 – A MLP network trained by Back Propagation rule

It is a supervised learning method, and it is an implementation of the Delta rule, Fig. 8, where as an example it is supposed to use sigmoidal activation function for all neurons of all layers. It requires a teacher that knows, or can calculate, the desired output for any given input. It is most useful for feed-forward networks (networks that have no feedback, or simply, that have no connections that loop). The term is an abbreviation for "backwards propagation of errors". Back Propagation requires that the activation function used by the artificial neurons (or "nodes") is differentiable. Main formulas are:

$$f(h) = \frac{1}{1+e^{-\sum_i w_{hi} f(i)}} \quad (3) \quad ; \quad f(j) = \frac{1}{1+e^{-\sum_h w_{jh} f(h)}} \quad (4)$$

$$\delta_h = f'(j)(Y - P(e)) \quad (5) \quad ; \quad \delta_i = f'(h)\sum w\delta_h \quad (6)$$

This document contains proprietary information of DAME project Board. All Rights Reserved.

$$w\_new_{jh} = w\_old_{jh} + \eta\delta_h f(j) + \alpha\Delta w\_old_{jh} \quad (7)$$
$$w\_new_{hi} = w\_old_{hi} + \eta\delta_i f(h) + \alpha\Delta w\_old_{hi} \quad (8)$$

Where:

- (3) and (4) are the activation function for a generic neuron of the, respectively, hidden layer and output layer. This is the mechanism to process and flow the input pattern signal through the "forward" or bottom-up phase (from input neuron layer up to output neuron layer);
- At the end of the "forward" phase the network error is calculated (inner argument of the (5)), to be used during the "backward" or top-down phase to modify (adjust) neuron weights;
- (5) and (6) are the descent gradient calculations of the "backward" phase, respectively, for a generic neuron of the output and hidden layer;
- (7) and (8) are the most important laws of the backward phase. They represent the weight modification laws, respectively, between output and hidden layers (7) and between hidden-input (or hidden-hidden if more than one hidden layer is present in the network topology) layers. The new weights are adjusted by adding to the old ones two terms:
    - $\eta\delta_h f(j)$: this is the descent gradient multiplied by a parameter, defined as "learning rate", generally chosen sufficiently small in [0, 1], in order to induce a smooth learning variation at each backward stage during training;
    - $\alpha\Delta w\_old_{jh}$: this is the weight variation multiplied by a parameter, defined as "momentum", generally chosen quite high in [0, 1], in order to give an high change to the weights to prevent the "local minima" occurrence problem during descent gradient training. When this "momentum" is non-zero the learning rule is considered a variation of standard Back Propagation, which foresees the "momentum" equal to zero;

These formulas are cyclically repeated during training. It is hence evident that the back propagation learning algorithm can be divided into two phases: bottom-up propagation and top-down weight update.

Phase 1: Propagation (forward)
Each propagation involves the following steps:

1. Forward propagation of a training pattern's input through the neural network in order to generate the propagation's output activations.
2. Back propagation of the propagation's output activations through the neural network using the training pattern's target in order to generate the deltas of all output and hidden neurons.

Phase 2: Weight Update (backward)
For each weight-synapse:

1. Multiply its output delta and input activation to get the gradient of the weight.
2. Bring the weight in the direction of the gradient by adding a ratio of it from the weight.

This ratio influences the speed and quality of learning; it is called the *learning rate*. The sign of the gradient of a weight indicates where the error is increasing, this is why the weight must be updated in the opposite direction.
Repeat the phase 1 and 2 until the you are satisfied with the performance of the network.

3.3.1.2 Generalization and statistics

In applications where the goal is to create a system that generalizes well in unseen examples, the problem of overtraining has emerged. This arises in over complex or over specified systems when the capacity of the network significantly exceeds the needed free parameters. There are two schools of thought for avoiding this problem: The first is to use cross-validation and similar techniques to check for the presence of overtraining and optimally select hyper parameters such as to minimize the generalization error. The second is to use

This document contains proprietary information of DAME project Board. All Rights Reserved.

some form of *regularization*. This is a concept that emerges naturally in a probabilistic (Bayesian) framework, where the regularization can be performed by selecting a larger prior probability over simpler models; but also in statistical learning theory, where the goal is to minimize over two quantities: the 'empirical risk' and the 'structural risk', which roughly corresponds to the error over the training set and the predicted error in unseen data due to overfitting.
Supervised neural networks that use an MSE (Mean Square Error) cost function can use formal statistical methods to determine the confidence of the trained model. The MSE on a validation set can be used as an estimate for variance. This value can then be used to calculate the confidence interval of the output of the network, assuming a normal distribution. A confidence analysis made this way is statistically valid as long as the output probability distribution stays the same and the network is not modified.
By assigning a softmax activation function on the output layer of the neural network (or a softmax component in a component-based neural network) for categorical target variables, the outputs can be interpreted as posterior probabilities. This is very useful in classification as it gives a certainty measure on classifications.

3.3.1.2.1 Cross Entropy

The MLP-BP also supports the use of ***Cross Entropy*** error function for addressing classification problems in a consistent statistical fashion, [A13].
Learning in the neural networks is based on the definition of a suitable error function, which is then minimized with respect to the weights and biases in the network. Error functions play an important role in the use of neural networks. A variety of different error functions exist.
For regression problems the basic goal is to model the conditional distribution of the output variables, conditioned on the input variables. This motivates the use of a sum-of-squares error function. But for classification problems the sum-of-squares error function is not the most appropriate choice. In the case of a 1-of-C coding scheme, the target values sum to unity for each pattern and so the network outputs will also always sum to unity. However, there is no guarantee that they will lie in the range [0,1].
In fact, the outputs of the network trained by minimizing a sum-of-squares error function approximate the posterior probabilities of class membership, conditioned on the input vector, using the maximum likelihood principle by assuming that the target data was generated from a smooth deterministic function with added Gaussian noise. For classification problems, however, the targets are binary variables and hence far from having a Gaussian distribution, so their description cannot be given by using Gaussian noise model.
Therefore a more appropriate choice of error function is needed.
Let us now consider problems involving two classes. One approach to such problems would be to use a network with two output units, one for each class. First let's discuss an alternative approach in which we consider a network with a single output y. We would like the value of y to represent the posterior probability $P(C_1 \mid x)$ for class C_1. The posterior probability of class C_2 will then be given by $P(C_2 \mid x) = 1 - y$.
This can be achieved if we consider a target coding scheme for which $t = 1$ if the input vector belongs to class C_1 and $t = 0$ if it belongs to class C_2. We can combine these into a single expression, so that the probability of observing either target value is $P(t \mid x) = y^t (1-y)^{1-t}$.
This equation is the equation for a binomial distribution known as Bernoulli distribution. With this interpretation of the output unit activations the likelihood of observing the training data set, assuming the data points are drawn independently from this distribution, is then given by

$$\prod_n (y^n)^{t^n} (1-y^n)^{1-t^n}$$

By minimizing the negative logarithm of the likelihood we get to the cross-entropy error function[6] in the form

[6] [Hopfield, 1987; Baum and Wilczek, 1988; Solla et al., 1988; Hinton, 1989; Hampshire and Pearlmutter, 1990]

This document contains proprietary information of DAME project Board. All Rights Reserved.

$$E = -\sum \left[t^n \ln y^n + (1-t^n) \ln(1-y^n) \right]$$

Let's consider some elementary properties of this error function. Differentiating this error function with respect to y^n we obtain

$$\frac{\partial E}{\partial y^n} = \frac{(y^n - t^n)}{y^n(1-y^n)} \quad \text{(a)}$$

The absolute minimum of the error function occurs when:

$$y^n = t^n \forall n$$

The considering network has one output whose value is to be interpreted as a probability, so it is appropriate to consider the logistic sigmoid activation function which has the property

$$g'(a) = g(a)(1-g(a)) \quad \text{(b)}$$

Combining equations (a) and (b) it can be seen that the derivative of the error with respect to *a* takes a simple form:

$$\delta^n \equiv \frac{\partial E}{\partial a^n} = y^n - t^n$$

This equation gives the error quantity which is back propagated through the network in order to compute the derivates of the error function with respect to the network weights. The same equation form can be obtained for the sum-of-squares error function and linear output units. This shows that there is a natural paring of error function and output unit activation function.
From the previous equations the value of the cross entropy error function at its minimum is given by

$$E_{\min} = -\sum \left[t^n \ln t^n + (1-t^n) \ln(1-t^n) \right] \quad \text{(c)}$$

The last equation becomes zero for 1-of-C coding scheme. However, when t^n is a continuous variable in the range (0,1) representing the probability of the input vector x^n belonging to class C, the error function is also the correct one to use, In this case the minimum value (c) of the error does not become 0. In this case it is appropriate by subtracting this value from the original error function to get a modified error function of the form

$$E = -\sum \left[t^n \ln \frac{y^n}{t^n} + (1-t^n) \ln \frac{(1-y^n)}{(1-t^n)} \right] \quad \text{(d)}$$

But before moving to cross-entropy for multiple classes let us describe more in detail its properties. Assume the network output for a particular pattern *n*, written in the form $y^n = t^n + e^n$.
Then the cross-entropy error function (d) can be transformed to the form

$$E = -\sum_n \left[t^n \ln \frac{\varepsilon^n}{t^n} + (1-t^n) \ln \left(1 - \frac{\varepsilon^n}{1-t^n} \right) \right] \quad \text{(e)}$$

So that the error function depends on the relative errors of the network outputs. Knowing that the sum of squares error function depends on the squares of the absolute errors, we can make comparisons. Minimization of the cross-entropy error function will tend to result in similar relative errors on both small

This document contains proprietary information of DAME project Board. All Rights Reserved.

and large target values. By contrast, the sum-of-squares error function tends to give similar absolute errors for each pattern, and will give large relative errors for small output values. This result suggests the better functionality of the cross-entropy error function over the sum-of-squares error function at estimating small probabilities. Another advantage over the sum-of-squares error function, is that the cross-entropy error function gives much stronger weight to smaller errors.

A particular case is the classification problem involving mutually exclusive classes, i.e. where the number of classes is greater than two. For this problem we should seek the form which the error function should take. The network now has one output y^k for each class, and target data which has a 1-of-c coding scheme, so that we have $t_k^n = b_{kl}$ for a pattern *n* from class C_l. The probability of observing the set of target values $t_k^n = b_{kl}$ given an input vector x^n is just $P(C_l \mid x) = y_l$.
Therefore the conditional distribution for this pattern can he written as

$$P(t^n \mid x^n) = \prod_{k=1}^{c} (y_k^n)^{t_k^n}$$

As before, starting from the likelihood function, by taking the negative logarithm, we obtain an error function of the form

$$E = -\sum_n \sum_{k=1}^{c} t_k^n \ln y_k^n \qquad \text{(f)}$$

For 1-of-C coding scheme the minimum value of the error function (f) equals 0. But the error function is still valid when t_k^n is a continuous variable in the range (0,1) representing the probability that x^n belongs to C_k.
To get the proper target variable the softmax activation function is used. So for the cross-entropy error function for multiple classes, equation (f), to be efficient the softmax activation function must be used.
By evaluating the derivatives of the softmax error function considering all inputs to all output units, (for pattern n) it can be obtained

$$\frac{\partial E^n}{\partial a_k} = y_k - t_k$$

which is the same result as found for the two-class cross-entropy error (with a logistic activation function). The same result is valid for the sum-of-squares error (with a linear activation function). This can be considered as an additional proof that there is a natural pairing of error function and activation function.
Clearly, for every activation function we get a proper error function, and as shown for the soft max activation function we must use the cross-entropy error function. It is obvious that by using non proper pairs of activation and error function the network would not perform as we would like to, giving results without sense.

3.3.1.3 MLP Practical Rules

The practice and expertise in the machine learning models, such as MLP, are important factors, coming from a long training and experience within their use in scientific experiments. The speed and effectiveness of the

This document contains proprietary information of DAME project Board. All Rights Reserved.

results strongly depend on these factors. Unfortunately there are no magic ways to a priori indicate the best configuration of internal parameters, involving network topology and learning algorithm.
But in some cases a set of practical rules to define best choices can be taken into account.

3.3.1.3.1 Selection of neuron activation function

- If there are good reasons to select a particular activation function, then do it
  - Mixture of Gaussian → Gaussian activation function;
  - Hyperbolic tangent;
  - Arctangent;
  - Linear threshold;
- General "good" properties of activation function
  - Non-linear;
  - Saturate – some max and min value;
  - Continuity and smooth;
  - Monotonicity: convenient but nonessential;
  - Linearity for a small value of net;
- Sigmoid function has all the good properties:
  - Centered at zero;
  - Anti-symmetric;
  - f(-net) = - f(net);
  - Faster learning;
  - Overall range and slope are not important;

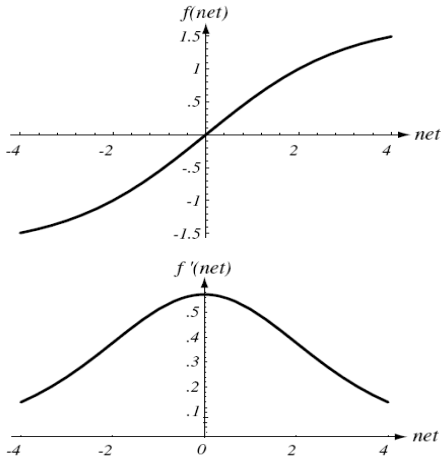


Fig. 9 – The sigmoid function and its first derivative

3.3.1.3.2 Scaling input and target values

- Standardize
  - Large scale difference
    - error depends mostly on large scale feature;
  - Shifted to Zero mean, unit variance
    - Need to be done once, before training;
    - Need full data set;
- Target value

This document contains proprietary information of DAME project Board. All Rights Reserved.

- Output is saturated
  - In the training, the output never reach saturated value;
    - Full training never terminated;
- Range [-1, +1] is suggested;

3.3.1.3.3 Number of hidden nodes

- Number of hidden units governs the expressive power of net and the complexity of decision boundary;
- Well-separated → fewer hidden nodes;
- From complicated density, highly interspersed → many hidden nodes;
- Heuristics rule of thumb:
  - More training data yields better result;
  - Number of weights < number of training data;
  - Number of weights ≈ (number of training data)/10;
  - Adjust number of weights in response to the training data:
    - Start with a "large" number of hidden nodes, then decay, prune weights…;

3.3.1.3.4 Number of hidden layers

- One or two hidden layers are OK, so long as differentiable activation function;
  - But one layer is generally sufficient;
- More layers → more chance of local minima;
- Single hidden layer vs double (multiple) hidden layer:
  - single is good for any approximation of continuous function;
  - double may be good some times;
- Problem-specific reason of more layers:
  - Each layer learns different aspects;

3.3.1.3.5 Initializing Weights

- Not to set zero – no learning take place;
  - Selection of good Seed for Fast and uniform learning;
  - Reach final equilibrium values at about the same time;
- For standardized data:
  - Choose randomly from single distribution;
  - Give positive and negative values equally $-\omega < w < +\omega$;
    - If ω is too small, net activation is small – linear model;
    - If ω is too large, hidden units will saturate before learning begins;

3.3.1.3.6 Momentum

- Benefit of preventing the learning process from terminating in a shallow local minimum;
  - α is the momentum constant;
  - converge if $0 \le |\alpha| \le 1$, typical value = 0.9;
  - α = 0: standard Back Propagation;

$$\mathbf{w}(m+1) = \mathbf{w}(m) + (1-\alpha)\Delta\mathbf{w}_{bp}(m) + \alpha\Delta\mathbf{w}(m-1)$$

This document contains proprietary information of DAME project Board. All Rights Reserved.

3.3.1.3.7 Learning rate

- Smaller learning-rate parameter makes smoother path;
- increase rate of learning yet avoiding danger of instability;
- First choice : $\eta \approx 0.1$;
- Suggestion : learning rate is inversely proportional to square root of the number of synaptic connection ($m^{-1/2}$) ;
- May change during training;

3.3.1.4 Implementation Details

The Multi Layer Perceptron (MLP) is one of the most common supervised neural architectures used in many application fields. It is especially related to classification and regression problems, and in DAME it is designed to be associated with such two functionality domains. In the following the details of its implementation is reported, together with practical information to configure the network architecture and the learning algorithm in order to launch and execute science cases and experiments.
The MLP with Back Propagation (MLP-BP) learning rule is designed starting from public library FANN[7] (Fast Artificial Neural Network), [A4, A14, A16]. FANN Library is a free open source neural network library, which implements multilayer artificial neural networks in C with support for both fully connected and sparsely connected networks. Cross-platform execution in both fixed and floating point are supported. It includes a framework for easy handling of training data sets. This library has been integrated to support a complete MLP-BP model for DAME scientific purposes.

For the user the MLP-BP system offers four use cases:

- **Train**
- **Test**
- **Run**
- **Full**

In the use case named "**Train MLP**", the software provides the possibility to train one ANN MLP. The user will be able to use new or existing (already trained) MLP weight configurations, adjust MLP parameters, set training parameters, set training dataset, manipulate the training dataset and execute the training.
There are several parameters to be set to achieve training, dealing with network topology and learning algorithm: training algorithm, error function, stop training function, desired error value, bit fail limit, learning moment, learning momentum, number of epochs for training, number of epochs between result reports. For details about their meaning, see section 4.7. Here we mention that the default values imposed in the source code for some parameters are:

- Error Tolerance (threshold optional parameter): 0.001;
- Number of iterations (optional parameter): 1000;
- Learning rate: 0.7;
- Learning momentum: 0;

A training dataset is a set of input and desired output vector couples. The user will have the option to: merge two different datasets, duplicate or subset dataset, shuffle data and scale the training data (see section 4.6.2 for details).

[7] http://leenissen.dk/fann/

This document contains proprietary information of DAME project Board. All Rights Reserved.

The following set of MLP parameters will be available: number of layers, number of neurons per layer, an array with weight values, activation function and activation steepness.
The software will use the selected training algorithm to train the specified MLP. During the training the error between desired and current output will be calculated, and the weights in the MLP will be updated. In addition the program saves the entire neural network in a file every time it hits a minimal error. In another file the program saves the MLP on predefined period, for example on every 100 epochs.
The training will stop in two cases:

- when the stop function reaches the desired error (defined by Error Tolerance parameter);
- when the maximum number of epochs is reached (defined by Number of Iterations parameter).

If at the end of the training the desired error is not reached the system will save the trained MLP that reached minimal error, otherwise it will save the MLP from the last epoch. Also the program will return a second file containing the MLP saved in the predefined period.
In case of the second use case "**Test MLP**", the tool provides the option to test an existing ANN MLP. The user will be able to specify an existing MLP, its parameters and its test dataset. A test dataset has the same structure as a train dataset (same number of columns input+targets). It can be specifically created for test purpose or it can be exactly the same of the training file. The program will forward propagate the input vectors from the dataset, calculating the error between the desired and the current outputs.
The third use case "**Run MLP**" will do a functional mapping from an input to an output vector, called forward propagation. The user will be able to specify input vector and adjust the MLP parameters. The program will forward propagate the input vector trough the MLP, will do the calculations and will give an output vector. In the Run case the input pattern file do not contain target columns.
The fourth use case "**Full MLP**" provides the possibility to train and test MLP at the same time. The user will be able to do the same activities as in the case of the "Train MLP" use case but he needs to specify the test dataset.
In all cases, if the MLP parameters are not set properly the software will automatically generate an error log and will alert the user.

During training it should be possible to use validation with the same or with different dataset from the training dataset. There are different ways to do the validation. Validating periodically the MLP will allow better control of the training and will try to avoid over fitting. When the validation is used the stop function is calculated from the validation results, meaning that the training end is conditioned from the validation errors instead of the training errors.
When the MLP is used in combination with Regression functionality, the default (hard-coded) neuron activation function used is the linear, while the user is able to choose between two **training modes**:

- MSE + BATCH: MSE means the standard Mean Square Error applied to the differences between network output and target. BATCH means that at each training cycle iteration the whole bundle of input patterns is submitted and propagated through the network before to adjust weights;
- MSE + INCREMENTAL: INCREMENTAL here means that at each iteration the network weights are adjusted immediately after each single input pattern submission;

When the MLP is used in combination with Classification functionality, the default (hard-coded) neuron activation function used is the sigmoid, while the user is able to choose between four **training modes**:

- MSE + BATCH: same as in the Regression case;
- MSE + INCREMENTAL: same as in the Regression case;
- CE + BATCH: CE means that the Cross Entropy method is applied to evaluate network output error;
- CE + INCREMENTAL;

This document contains proprietary information of DAME project Board. All Rights Reserved.

Concerning **the output files**, their type and quantity depends on the use case:

- **Training:**
  - *outputFileName.tra*: CSV format train output file;
  - *outputFileName.ERROR*: ASCII format (simple txt) error log file;
  - *outputFileName.csv.jpg*: JPEG format error value scatter plot;
  - *outputFileName.csv*: CSV format error output file;
  - *outputFileName.log*: ASCII format (simple txt) experiment log file;
  - *outputFileName_netTmp.mlp*: MLP network temporary file;
  - *outputFileName_netTrain.mlp*: trained weight matrix file;

- **Test**:
  - outputFileName.ERROR: ASCII format (simple txt) error log file;
  - outputFileName.tes: CSV format test output file;
  - outputFileName.log: ASCII format (simple txt) experiment log file;
  - outputFile Name.tes.ascii.matrix: (only for Classification) ASCII format (simple txt) confusion matrix report file;
  - outputFileName.tes.jpg: (only for Regression) JPEG format test scatter plot;

- **Full:**
  - the sum of Training and Test output files;

- **Run:**
  - outputFileName.ERROR: ASCII format (simple txt) error log file;
  - outputFileName.run: CSV format run output file;
  - outputFileName.log: ASCII format (simple txt) experiment log file;

This document contains proprietary information of DAME project Board. All Rights Reserved.

4 The Data Mining Suite User's Manual

The DAME Program includes many services and applications and it is foreseen to grow up its features and available tools in a fast and heterogeneous way. In the following a deep description of all already available resources is performed (alpha release).

Data Mining is usually conceived as an application (deterministic/stochastic algorithm) to extract unknown information from noisy data, [R4]. This is basically true but in some way it is too much reductive with respect to the wide range covered by mining concept domains. More precisely, in DAME, data mining is intended as techniques of exploration on data, based on the combination between parameter space filtering, machine learning, soft computing techniques associated to a functional domain. The functional domain term arises from the conceptual taxonomy of research modes applicable on data, in which the various machine learning methods (statistical and analytical models and algorithms) can be applied to explore data under a particular aspect, according to the associated functionality scope (section 3.2).

In the DAME terminology we use the following terms with the particular meaning:

- **DM model**: one of the data mining models integrated in the Suite. It can be either a supervised machine learning algorithm or an unsupervised one, depending on the available data BoK and the scientific target of the user experiment;
- **Functionality**: one of the functional domains in which the user wants to explore the available data (for example, regression, classification or clustering). The choice of the functionality target can limit the choice of the DM model to be associated;
- **Experiment**: it is the scientific pipeline (including optional pre-processing or preparation of data) that it includes the choice of a combination of DM model and a functionality;
- **Use Case**: for each DM model there are exposed to the user different running cases of the chosen model, that can be executed singularly or in a prefixed workflow sequence. The model usually includes training, test, validation and run use cases, in order to, respectively, perform learning, verification, validation and execution phases. In most cases there is also the "full" use case, that automatically executes all of listed cases as a whole sequence.

The DAME design architecture is implemented by following standard LAR (Layered Application Architecture) strategy, which foresees a software system based on a layered logical structure, where different layers (composed by internal components) communicate with each other with simple and well-defined rules, Fig. 10:

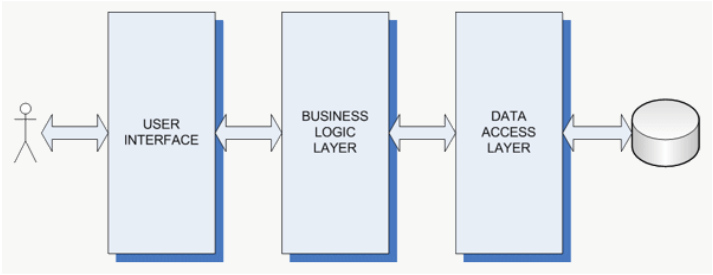


Fig. 10 – Typical Layered Application Architecture

- ✓ Data Access Layer (DAL): the persistent data management layer, responsible of the data archiving system, including consistency and reliability maintenance;

This document contains proprietary information of DAME project Board. All Rights Reserved.

- ✓ Business Logic Layer (BLL): the core of the system, responsible of the management of all services and applications implemented in the infrastructure, including information flow control and supervision;
- ✓ User Interface (UI): responsible of the interaction mechanisms between the BLL and users, including data and command I/O and views rendering.

In the Alpha release, the models and functionalities available are listed in the following table.

MODEL	CATEGORY	FUNCTIONALITY
MLP + Back Propagation learning rule	Supervised	Classification, Regression

Tab. 1 – The DM models available in DAME alpha release

The MLP is one of the models that can be used in combination with more than one (two) functionalities. For such model there are instanced two different plugins in the Suite, one for each couple model-functionality (i.e. Classification-MLP and Regression-MLP).

4.1 Overview

Main philosophy behind the interaction between user and the DMS (Data Mining Suite) is the following.
The DMS is organized under the form of working sessions (hereinafter named workspaces) that the user can create, modify and erase. You can imagine the entire DMS as a container of services, hierarchically structured as in Fig. 11. The user can create as many workspaces as desired. Each workspace is enveloping a list of data files and experiments, the latter defined by the combination between a functionality domain and a series (one at least) of data mining models. In principle there should be many experiments belonging to a single workspace, made by fixing the functional domain and by slightly different variants of a model setup and configuration or by varying the associated models.

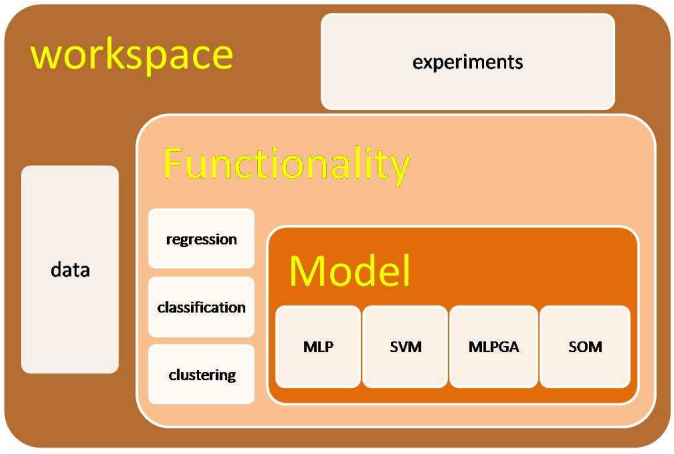


Fig. 11 – Suite functional hierarchy

By this way, as usual in data mining, the knowledge discovery process should basically consist of several experiments belonging to a specified functionality domain, in order to find the model, parameter configuration and dataset (parameter space) choices that give the best results (in terms of performance and reliability). The following sections describes in detail the practical use of the DMS from the end user point of view. Moreover, the DMS has been designed to build and execute a typical complete scientific pipeline

This document contains proprietary information of DAME project Board. All Rights Reserved.

(hereinafter named workflow) making use of machine learning models. This specification is crucial to understand the right way to build and configure data mining experiment with DMS.
In fact, machine learning algorithms (hereinafter named models) need always a pre-run stage, usually defined as training (or learning phase) and are basically divided into two categories: supervised and unsupervised models, depending, respectively, if they make use of a base of knowledge (couples input/target output for each datum) to perform training or not.
So far, any scientific workflow must take into account the training phase inside its operation sequence.
Apart from the training step, a complete scientific workflow always includes a well-defined sequence of steps, including pre-processing (or equivalently preparation of data), training, validation, run, and in some cases post-processing.

The DMS permits to perform a complete workflow, having the following features:

- A workspace to envelope all input/output resources of the workflow;
- A dataset editor, provided with a series of pre-processing functionalities to edit and manipulate the raw data uploaded by the user in the active workspace (see section 4.6 for details);
- The possibility to copy output files of an experiment in the workspace to be arranged as input dataset for subsequent execution (the output of training phase should become the input for the validate/run phase of the same experiment);
- An experiment setup toolset, to select functionality domain and machine learning models to be configured and executed;
- Functions to visualize graphics and text results from experiment output;
- A plugin-based toolkit to extend DMS functionalities and models with user own applications;

4.2 User Registration and Access[8]

The DMS makes use (embedded to the end user) of the Cloud computing infrastructure, made by single PCs in combination with GRID resources. This requires a reliable level of security in order to launch jobs (experiments) in a safe and coordinated way. This level of security is obtained by an accounting procedure that foresees an initial registration for new users, in order to activate their account on the DAME Suite. After activation, all subsequent accesses will require login and password, as defined by the user at the registration stage.
The registration form requires the following information to be filled in by the user:

- Name: first name of the user;
- Surname: Family name of the user;
- User e-mail: the user e-mail (it will become his access login). It is important to define a real address, because it will be also used by the DMS for communications, feedbacks and activation instructions;
- Country: country of the user;
- Affiliation: the institute/academy/society of the user;
- Password: a safe password (at least 6 chars, as mandatory), without spaces and special chars;

After registered the user can access to the webapp by inserting proper account information in the user login entry page, Fig. 12.

[8] The registration procedure and related features are not available in the alpha release

This document contains proprietary information of DAME project Board. All Rights Reserved.

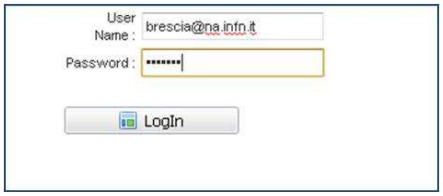


Fig. 12 – The user login form to access at the web application

After authentication the home page of the webapp is shown in Fig. 13.

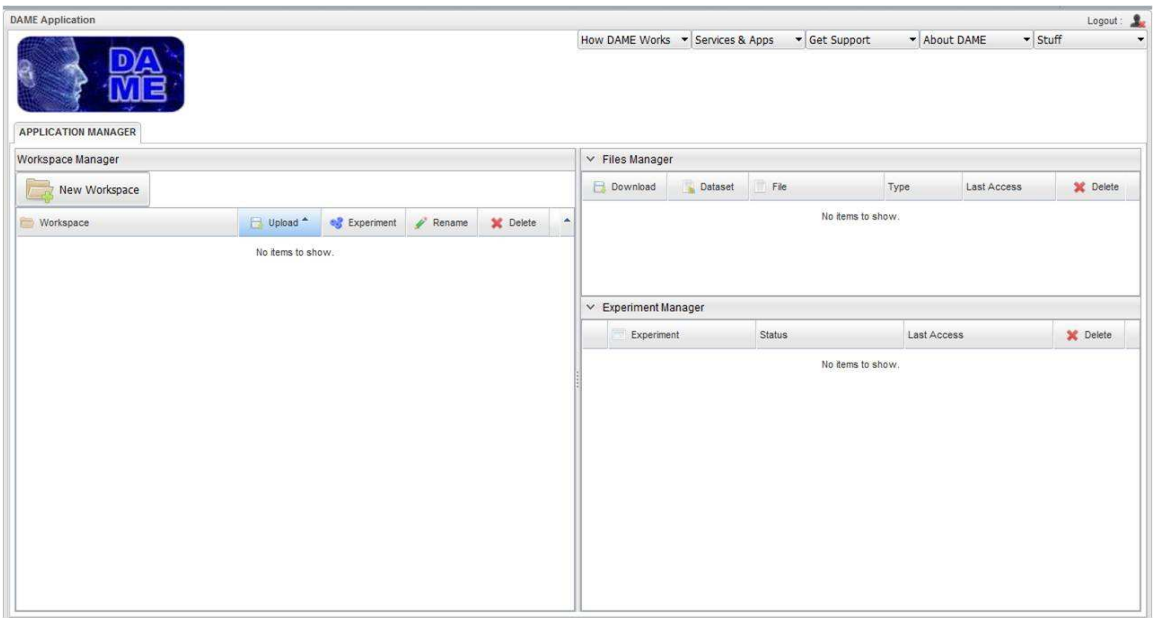


Fig. 13 – The Web Application starting page (home)

4.3 The command icons

The interaction between user and GUI is based on the selection of icons, which correspond to basic features available to perform actions. Here their description, related to the red circles in Fig. 14 is reported:

1. **The header menu options**. When selected, a pop submenu is showed with some options;
2. **Logout button**. If pressed the GUI (and related working session) is closed;
3. **Operation tabs**. The GUI is organized like a multi-tab browser. Different tabs are automatically open when user wants to edit data file to create datasets, to upload files or to configure and launch experiments;
4. **Creation of new workspaces**. When selected and named, the new workspace appears in the Workspace List Area (Workspace sub window);
5. **Upload command**. When selected, the user is able to select a new file to be uploaded into the Workspace Data Area (Files Manager sub window). The file can be uploaded from external URI or from local (user) HD;
6. **Creation of new experiment**. When selected, the user is able to create a new experiment (a specific new tab is open to configure and launch the experiment);
7. **Rename workspace command**. When selected the user can rename the workspace;

This document contains proprietary information of DAME project Board. All Rights Reserved.

8. **Delete Workspace command**. When selected, the user can delete the related workspace (only if no experiments are present, otherwise the system alerts you to empty the workspace before to erase it);
9. **Download command**. When selected the user can download locally (on his HD) the selected file;
10. **Dataset Editor command**. When selected a new tab is open, where the user can create new dataset files, starting from the original data file selected, by using all dataset manipulation features;
11. **Delete file command**. When selected the user can delete the selected file from current workspace;
12. **Experiment verbose list command**. When selected the user can open the experiment file list (for experiment in ended state) in a verbose mode, showing all related files created and stored;
13. **Download experiment file command**. When selected the user can download locally (on his HD) the related experiment file;
14. **AddinWS command**. When selected, the related file is automatically moved from experiment file list to the currently active workspace file list (Files Manager sub window). This feature is useful to re-use an output file of a previous experiment as input file of a new experiment;

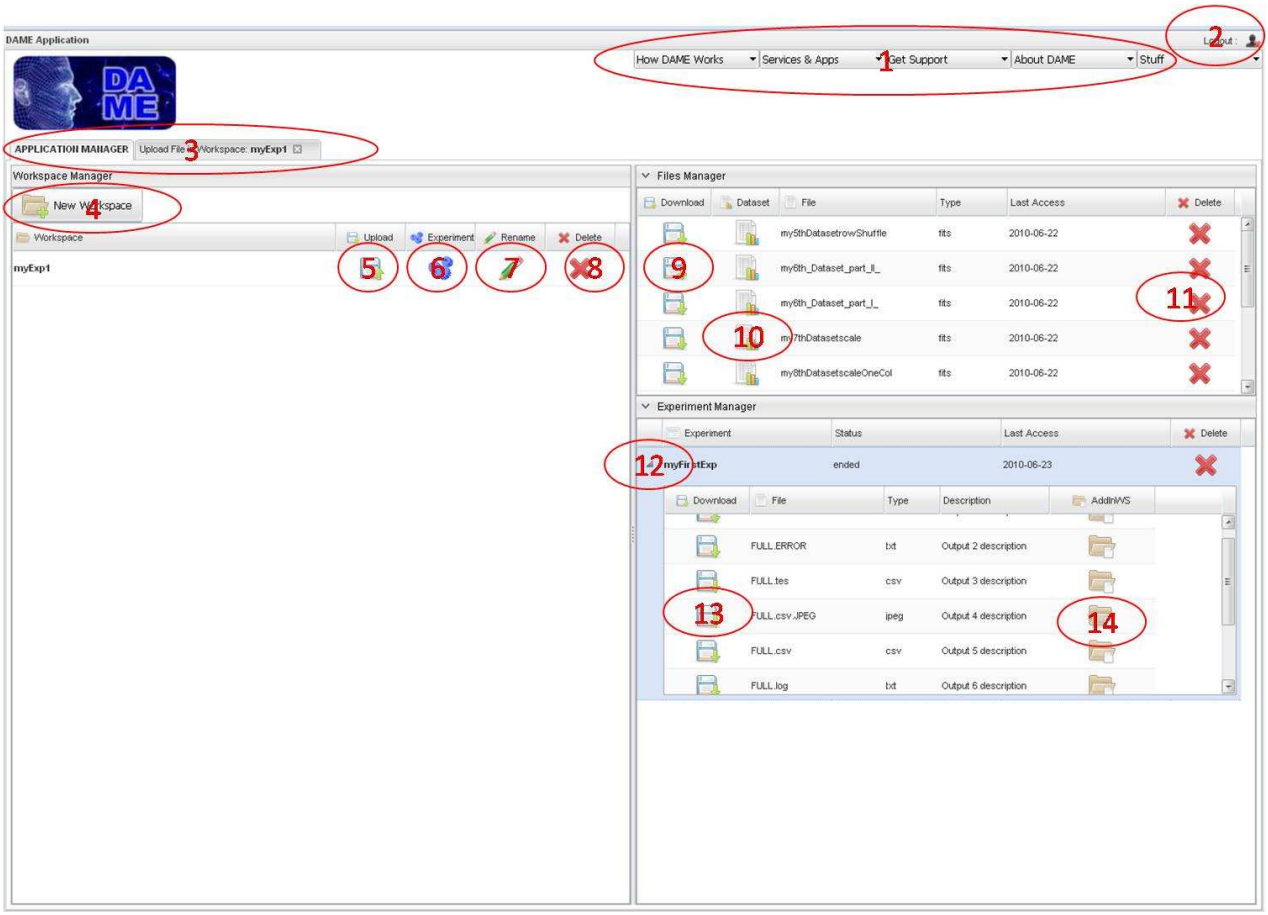


Fig. 14 – The Web Application main commands

4.4 Workspace Management

A workspace is namely a working session, in which the user can enclose resources related to scientific data mining experiments. Resources can be data files, uploaded in the workspace by the user, files resulting from some manipulations of these data files, i.e. dataset files, containing subsets of data files, selected by the user as input files for his experiments, eventually normalized or re-organized in some way (see section 4.6 for

This document contains proprietary information of DAME project Board. All Rights Reserved.

details). Resources can also be output files, i.e. obtained as results of one or more experiments configured and executed in the current "active" workspace (see section 4.7 for details).
The user can create a new or select an existing workspace, by specifying its name. After opening the workspace, this automatically becomes the "active" workspace. This means that any further action, manipulating files, configuring and executing experiments, upload/download files, will result in the active workspace, Fig. 15. In this figure it is also shown the right sequence of main actions in order to operate an experiment (workflow) in the correct way.

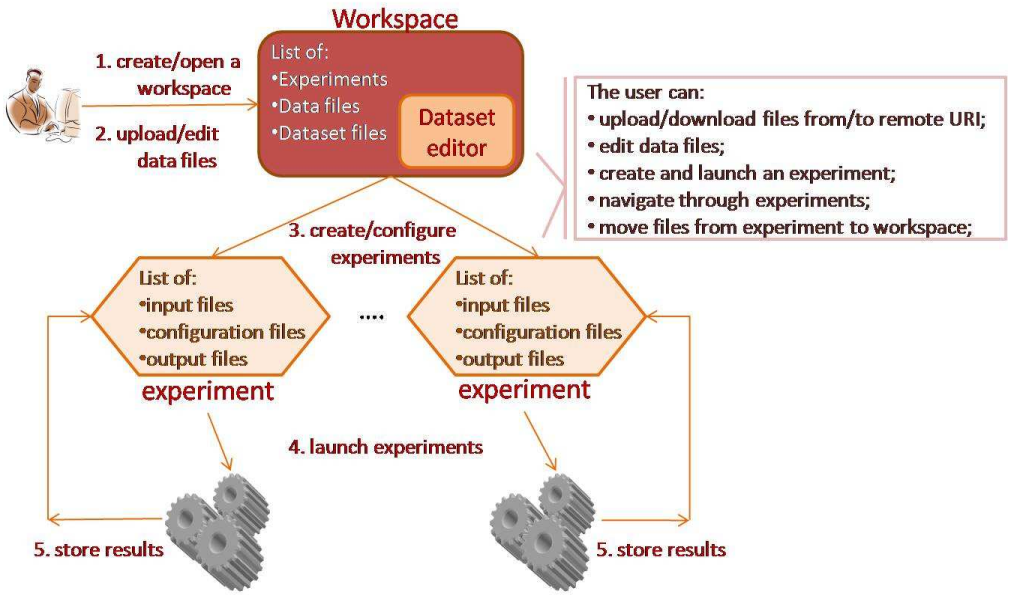


Fig. 15 – The right sequence to configure and execute an experiment workflow

So far, the basic role of a workspace is to make easier to the user the organization of experiments and related input/output files. For example the user could envelope in a same workspace all experiments related to a particular functionality domain, although using different models.
It is always possible to move (copy) files from experiment to workspace list, in order to re-use a same dataset file for multiple experiment sessions, i.e. to perform a workflow.

After access, the user must select the "active" workspace. If no workspaces are present, the user must create a new one, otherwise the user must select one of the listed workspace. The user can always create a new workspace by pressing the button as in Fig. 16.

Fig. 16 – the button "New Workspace" at left corner of workspace manager window

As consequence the user must assign a name to the new workspace, by filling in the form field as in Fig. 17.

This document contains proprietary information of DAME project Board. All Rights Reserved.

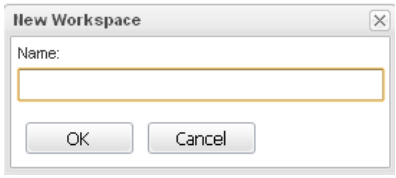


Fig. 17 – the form field that appears after pressing the "New Workspace" button

After creation, the active workspace can be populated by data and experiments, Fig. 18.

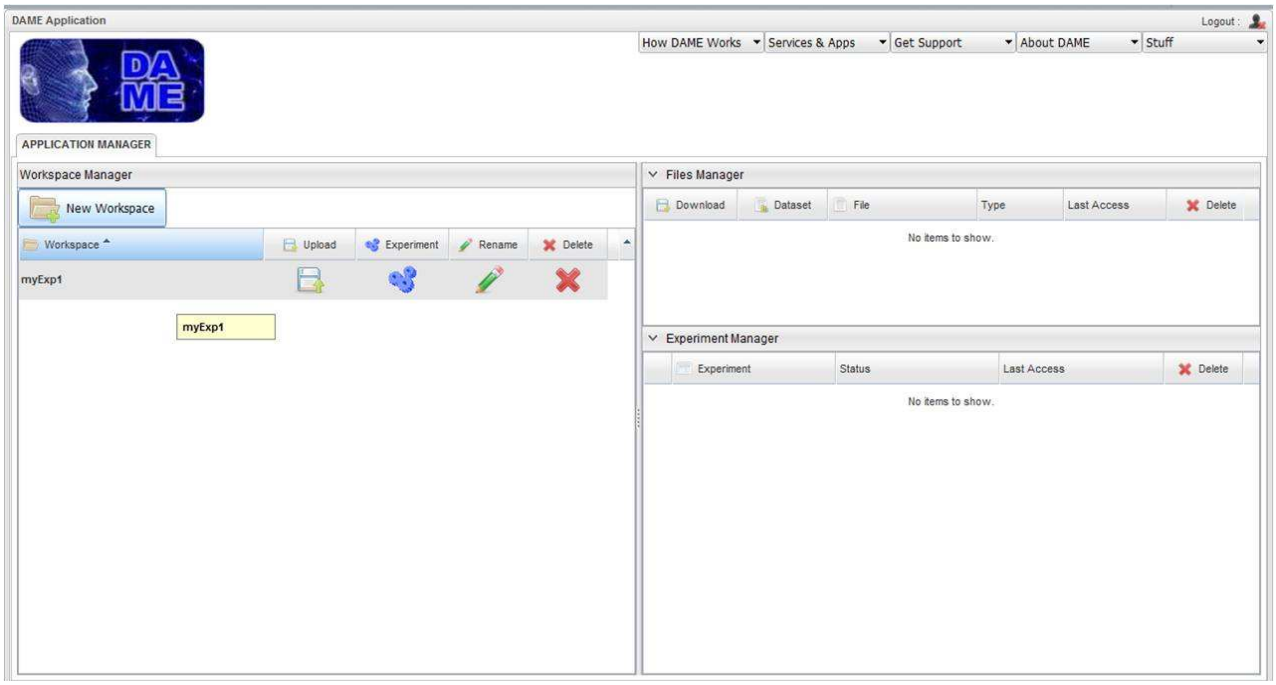


Fig. 18 – the active workspace created in the Workspace List Area

The GUI is organized as a classical modern browser, divided into specific functional areas (see Fig. 13). Main areas of the GUI are the following:

- Header Area (HA): the top page segment, containing the program logo and a series of persistent options related with documentation and information available online or addressable at specific DAME website pages.
- Workspace List Area (WLA): where the list of user defined workspaces appears, with some options useful to handle workspaces;
- Workspace Data Area (WDA): when a workspace is selected, here the list of its files, raw data uploaded by user, dataset files and intermediate files of past experiments, appears. There are specific options to manipulate the files;
- Data Editor Area (DEA): this is shown as a new tab in the DMS browsing page, open on request by the user (i.e. when the option "Edit" is selected for a related selected file). This tab hosts a series of manipulating functions (described in detail in the section 4.6) to create proper dataset from raw data files, previously uploaded by the user;
- Experiment Area (EA): where all experiments, created in the active workspace, are listed, with their current operational status and specific options;
- Experiment Data Area (EDA): when one experiment is selected in the EA, the list of related data (input, configuration, log, output files) appears, with some options to handle them;

This document contains proprietary information of DAME project Board. All Rights Reserved.

- Experiment Configuration Area (ECA): tab open when the user selects the option to prepare and execute an experiment. It includes the functionality and model selection, model parameter setup, input data file names.

This document contains proprietary information of DAME project Board. All Rights Reserved.

4.5 Header Area

At the top segment of the DMS GUI there is the so-called Header Area. Apart from the DAME logo, it includes a persistent menu of options directly related to information and documentation (this document also) available online and/or addressable through specific DAME program website pages.

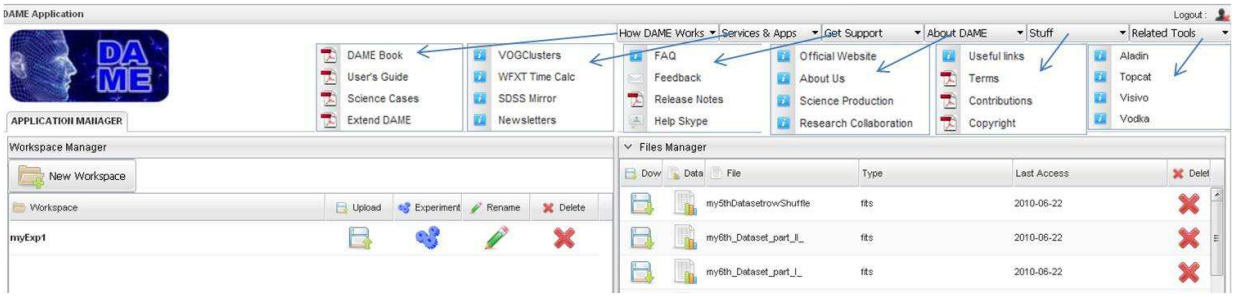


Fig. 19 – The GUI Header Area with all submenus open

The options are described in the following table (Tab. 2).

OPTION NAME	CATEGORY	DESCRIPTION
DAME Book	How DAME Works	The program Book
User's Guide		Guidelines of the GUI
Science Cases		document on experiment configuration "how to"
Extend DAME		document on plugin toolset
VOGClusters	Services & Apps	Description and link information of the DAME service related to the globular clusters text and data mining
WFXT Time Calc		Description and link information of the DAME service related to the WFXT Time Calculator
SDSS Mirror		Description and link information of the DAME service related to the local mirror of SDSS archive
Newsletters		Link to the DAME Newsletters download page
FAQ	Get Support	Frequently Asked Questions (link a web page)
Feedback		send a feedback to DAME Working group
Release Notes		Technical Notes about past and last releases of the DMS
Help Skype		Skype helpdesk: (help dame)
Official Website	About DAME	Link to DAME Program official website
About Us		Link to website dedicated page
Science Production		Link to website dedicated page
Research Collaboration		Link to website dedicated page
Useful Links	Stuff	Link to website dedicated page
Terms		Download specific document
Contributions		Download specific document
Copyright		Download specific document
Topcat	Related Tools	Link to project website
Aladin		Link to project website
Vodka		Link to project website
Visivo		Link to project website

Tab. 2 – Header Area Menu Options[9]

[9] Some header menu options are not available in the alpha release

This document contains proprietary information of DAME project Board. All Rights Reserved.

4.6 Data Management

The Data are the heart of the web application (data mining & exploration). All features directly or not are involved within the data manipulation. So far, a special care has been devoted to features giving the opportunity to upload, download, edit, transform, submit, create data.
In the GUI input data (i.e. candidates to be inputs for scientific experiments) are basically belonging to a workspace (previously created by the user). All these data are listed in the "Files Manager" sub window. These data can be in one of the supported formats, i.e. data formats recognized by the web application as correct types that can be submitted to machine learning models to perform experiments. They are:

- **FITS (tabular .fits files);**
- **ASCII (.txt or .dat ordinary files);**
- **VOTable (VO compliant XML document files);**
- **CSV (Comma Separated Values .csv files);**

The user has to pay attention to use input data in one of these supported formats in order to launch experiments in a right way.

Other types are permitted but not as input to experiments. For example, log, jpeg or "not supported" text files are generated as output of experiments, but only supported types can be eventually re-used as input data for experiments.
There is an exception to this rule for file format with extension **.ARFF (Attribute Relation File Format)**. These files can be uploaded and also edited by dataset editor, by using the type "CSV". But their extension .ARFF is considered "unsupported" by the system, so you can use any of the dataset editor options to change the extension (automatically assigned as CSV). Then you can use such files as input for experiments.
These output file are generally listed in the "Experiment Manager" sub window, that can be verbosely open by the user by selecting any experiment (when it is under "ended" state).
Other data files are created by dataset creation features, a list of operations that can be performed by the user, starting from an original data file uploaded in a workspace. These data files are automatically generated with a special name as output of any of the manipulation dataset operations available.
Confused? Well, don't panic please. Let's read carefully next sections.

4.6.1 Upload user data

As mentioned before, after the creation of at least one workspace, the user would like to populate the workspace with data to be submitted as input for experiments. Remember that in this section we are dealing with supported data formats only!

Fig. 20 – The Upload data feature open in a new tab

This document contains proprietary information of DAME project Board. All Rights Reserved.

As shown in Fig. 20, when the user selects command icon nr. 5, showed in the Fig. 14, a new tab appears. The user can choose to upload his own data file from, respectively, from any remote URI (well known...!) or from his local Hard Disk.
In the first case (upload from URI[10]), the Fig. 21 shows how to upload a supported type file from a remote address.

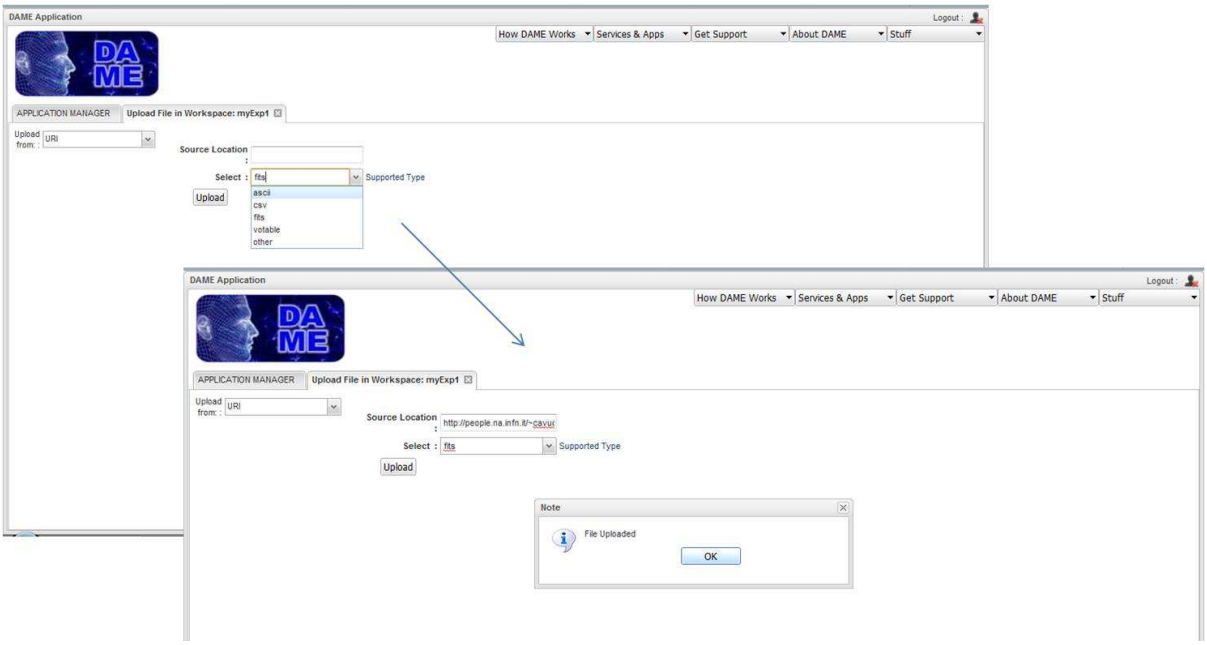


Fig. 21 – The Upload data from external URI feature

In the second case (upload from Hard Disk) the Fig. 22 shows how to select and upload any supported file in the GUI workspace from the user local HD.

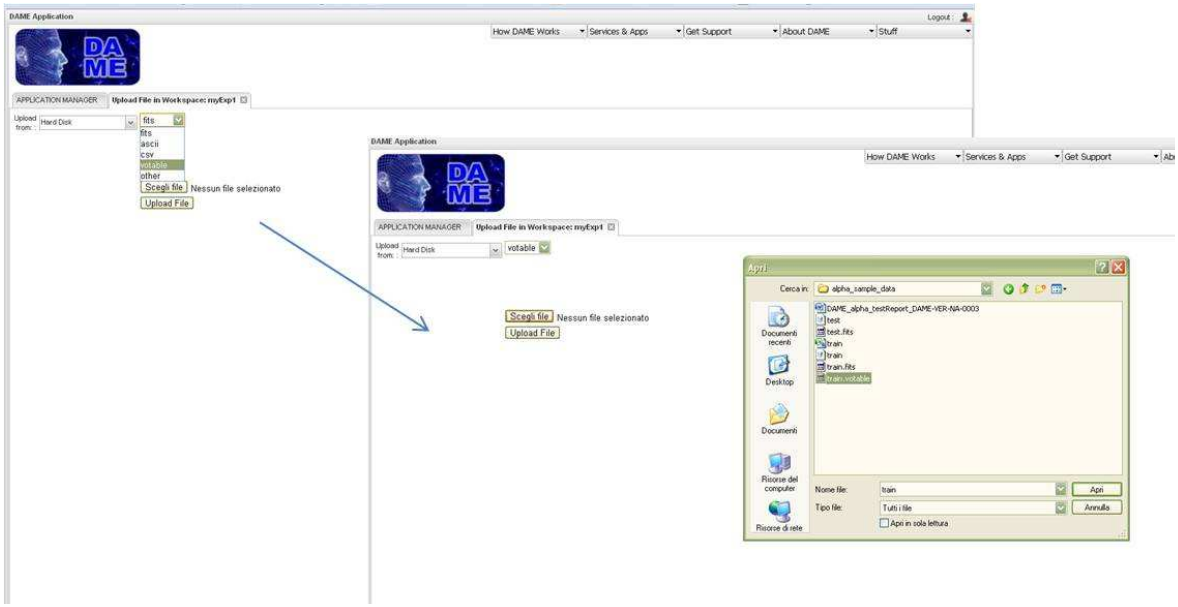


Fig. 22 – The Upload data from Hard Disk feature

[10] For example from the DAME website specific utility page at URI: http://voneural.na.infn.it/alpha_info.html

This document contains proprietary information of DAME project Board. All Rights Reserved.

After the execution of the operation, coming back to the main GUI tab, the user will found the uploaded file in the “Files Manager” sub window related with the currently active workspace, Fig. 23.

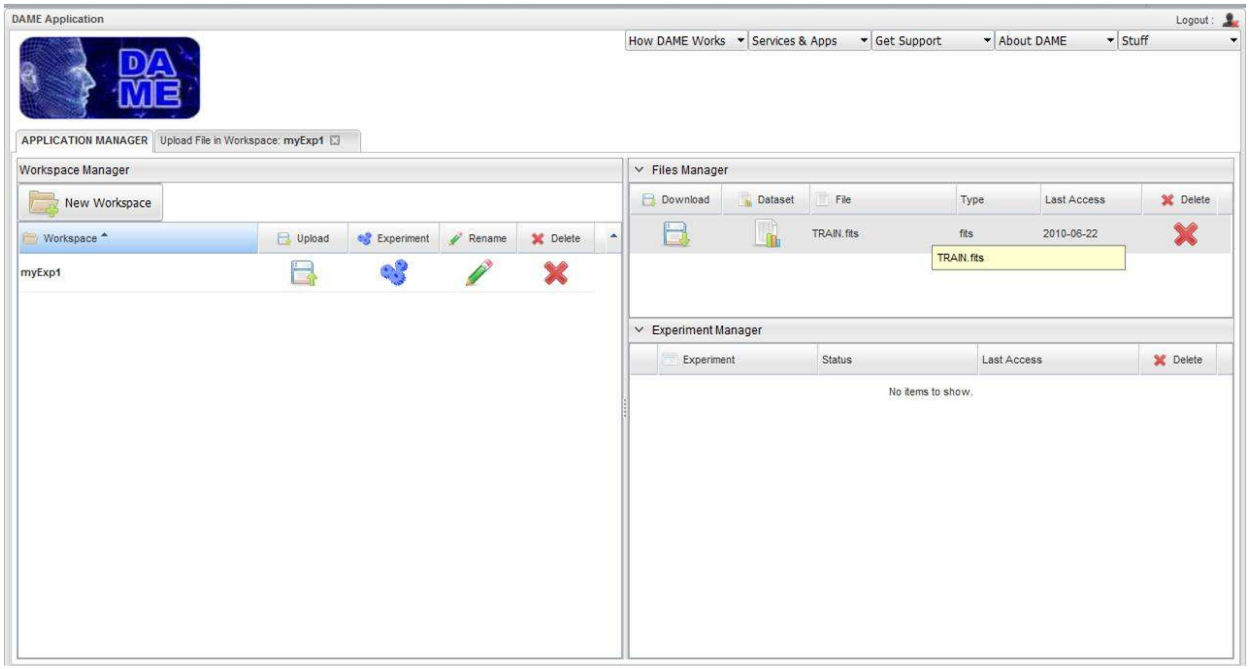


Fig. 23 – The Uploaded data (train.fits) in the Files Manager sub window

4.6.2 Create dataset files

If the user has already uploaded any supported data file in the workspace, it is possible to select it and to create datasets from it. This is a typical pre-processing phase in a machine learning based experiment, where, starting form an original data file, several different files must be prepared and provided to be submitted as input for, respectively, training, test and validate the algorithm chosen for the experiment. This pre-processing is generally made by applying one or more modification to the original data file (for example obtained from any astronomical observation run or cosmological simulation). The operations available in the web application are the following, Fig. 24:

- **Feature Selection;**
- **Columns Ordering;**
- **Sort Rows by Column;**
- **Column Shuffle;**
- **Row Shuffle;**
- **Split by Rows;**
- **Dataset Scale;**
- **Single Column scale;**

All these operations, one by one, can be applied starting from a selected data file uploaded in the currently active workspace.

This document contains proprietary information of DAME project Board. All Rights Reserved.

DAME Application
How DAME Works
Services & Apps
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Configuration
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.

Fig. 24 – The dataset editor tab with the list of available operations

4.6.2.1 Feature Selection

This dataset operation permits to select and extract arbitrary number of columns, contained in the original data file, by saving them in a new file (of the same type and with the same extension of the original file), named as <user selected name>columnSubset (i.e. with specific suffix *columnSubset*). This function is particularly useful to select training columns to be submitted to the algorithm, extracted from the whole data file. Details of the simple procedure are reported in Fig. 25, Fig. 26 and Fig. 27.

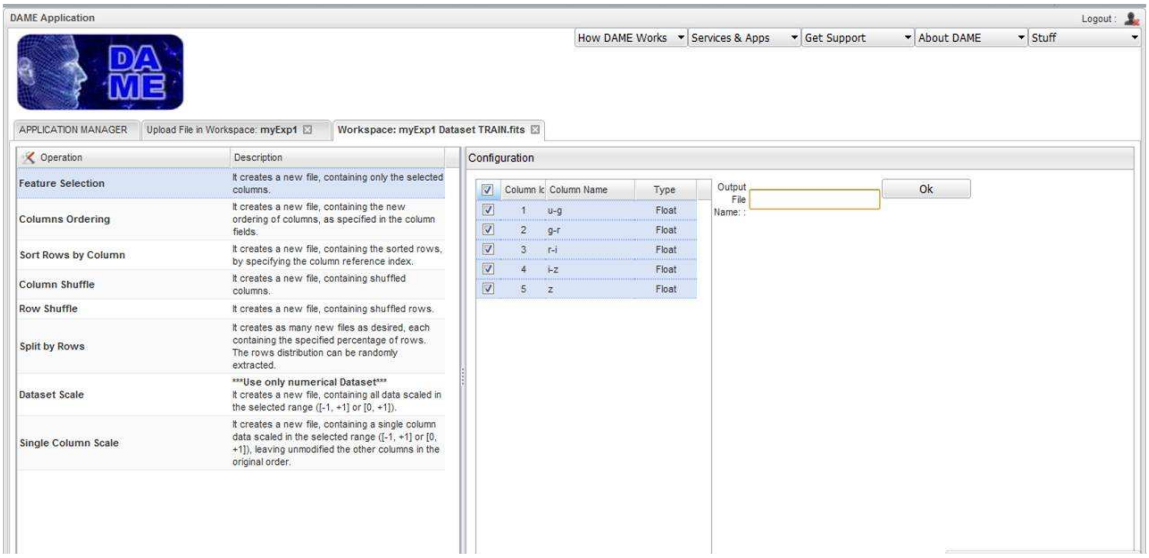

DAME Application
Logout :
How DAME Works
Services & Apps
Get Support
About DAME
Stuff
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Configuration
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Output File Name: :
Ok

Fig. 25 – The Feature Selection operation – step 1

This document contains proprietary information of DAME project Board. All Rights Reserved.

As clearly visible in Fig. 25, the *Configuration* panel shows the list of columns originally present in the input data file, that can be selected by proper check boxes. Note that the whole content of the data file (in principle a massive data set) is not shown, but simply labelled by column meta-data (as originally present in the file).

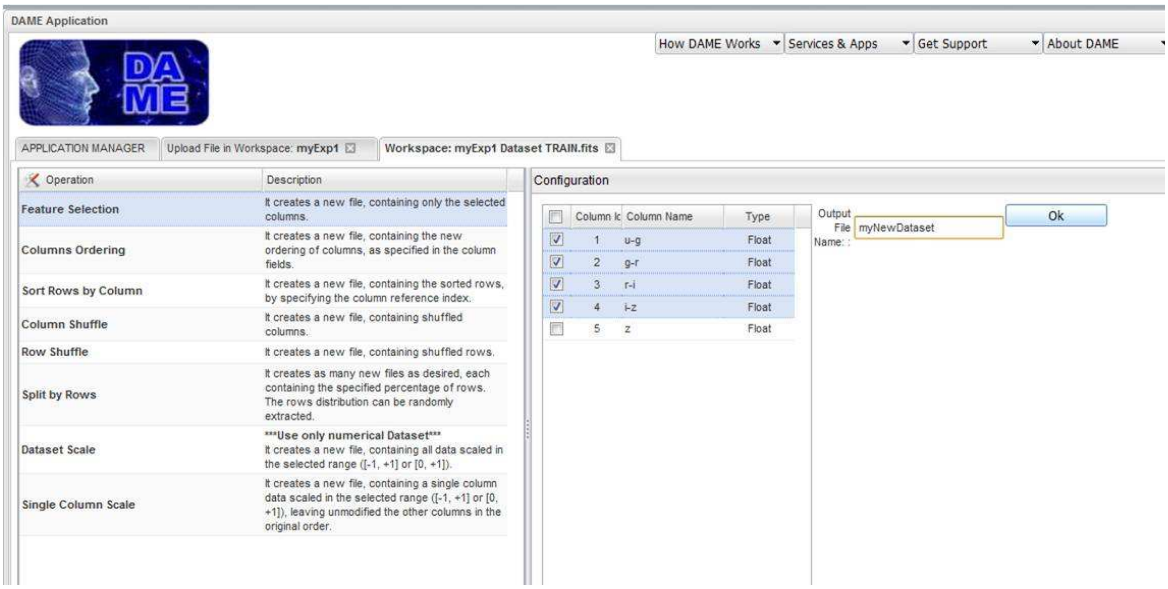

DAME Application
How DAME Works
Services & Apps
Get Support
About DAME
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Output File Name:
myNewDataset
Ok

Fig. 26 – The Feature Selection operation – step 2

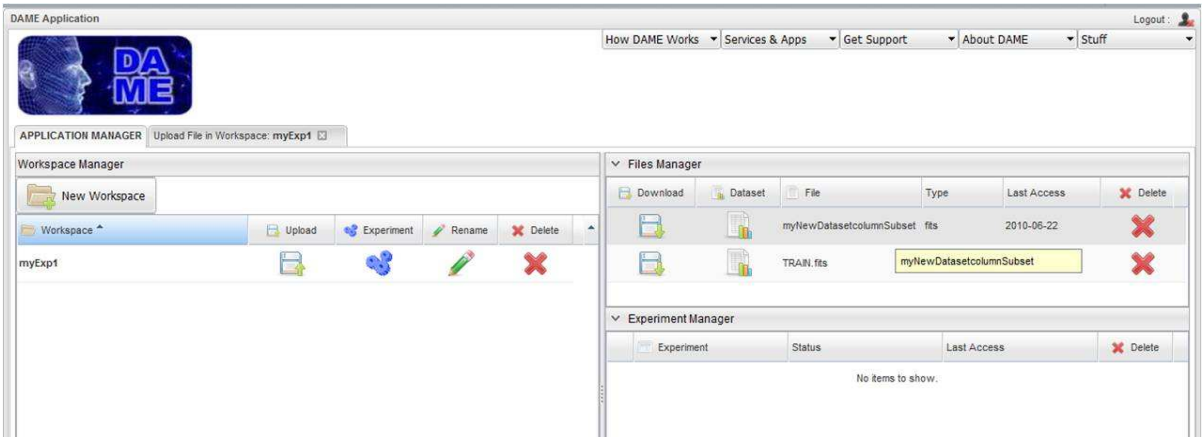


Fig. 27 – The Feature Selection operation – the new file created

4.6.2.2 Column Ordering

This dataset operation permits to select an arbitrary order of columns, contained in the original data file, by saving them in a new file (of the same type and with the same extension of the original file), named as <user selected name>columnSort (i.e. with specific suffix *columnSort*). Details of the simple procedure are reported in Fig. 28, Fig. 29 and Fig. 30.

This document contains proprietary information of DAME project Board. All Rights Reserved.

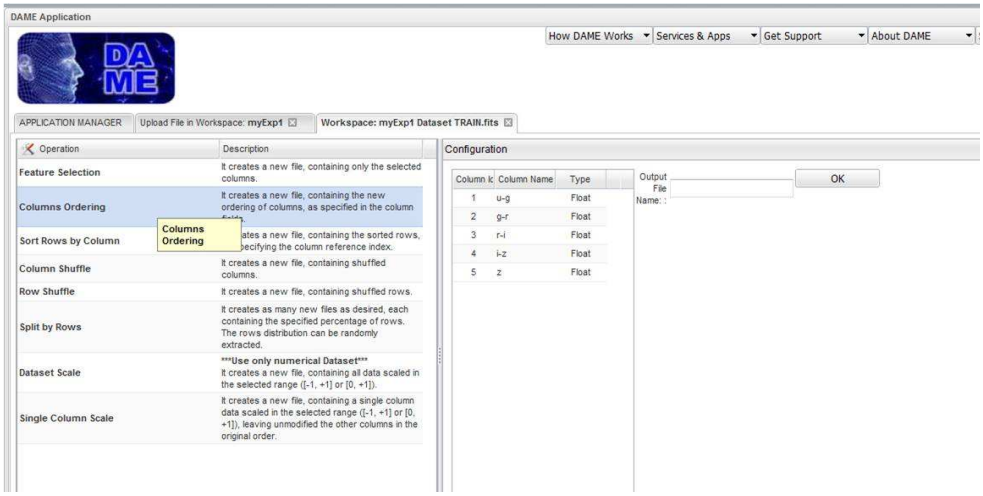

DAME Application
How DAME Works
Services & Apps
Get Support
About DAME
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column
Sort Rows by Column
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Output File Name:
OK

Fig. 28 – The Column Ordering operation – step 1

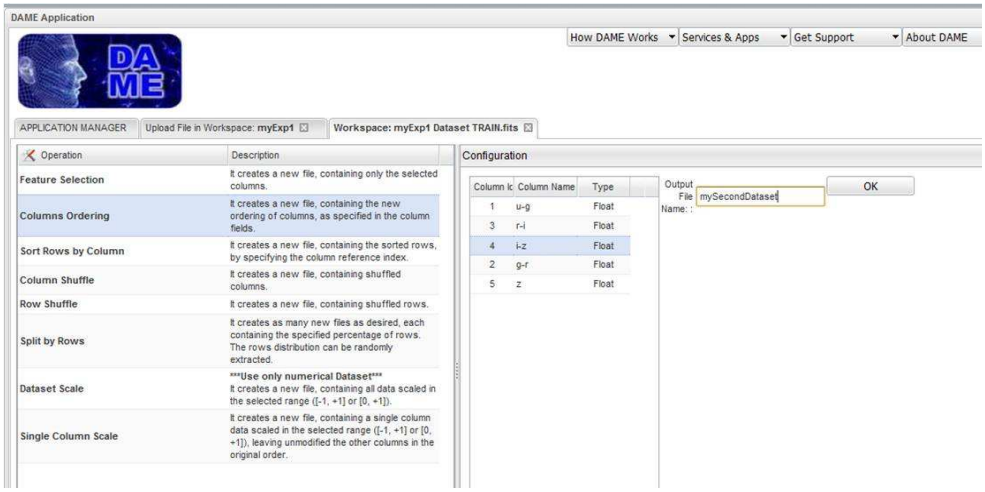


Fig. 29 – The Column Ordering operation – step 2

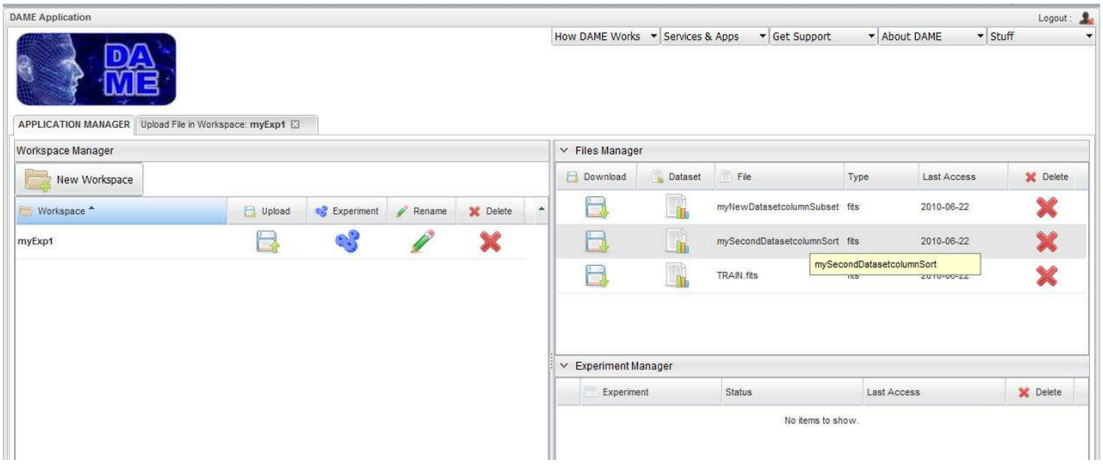


Fig. 30 – The Column Ordering operation – the new file created

This document contains proprietary information of DAME project Board. All Rights Reserved.

4.6.2.3 Sort Rows by Column

This dataset operation permits to select an arbitrary column, between those contained in the original data file, as sorting reference index for the ordering of all file rows. The result is the creation of a new file (of the same type and with the same extension of the original file), named as <user selected name>rowSort (i.e. with specific suffix *rowSort*). Details of the simple procedure are reported in Fig. 31, Fig. 32 and Fig. 33.

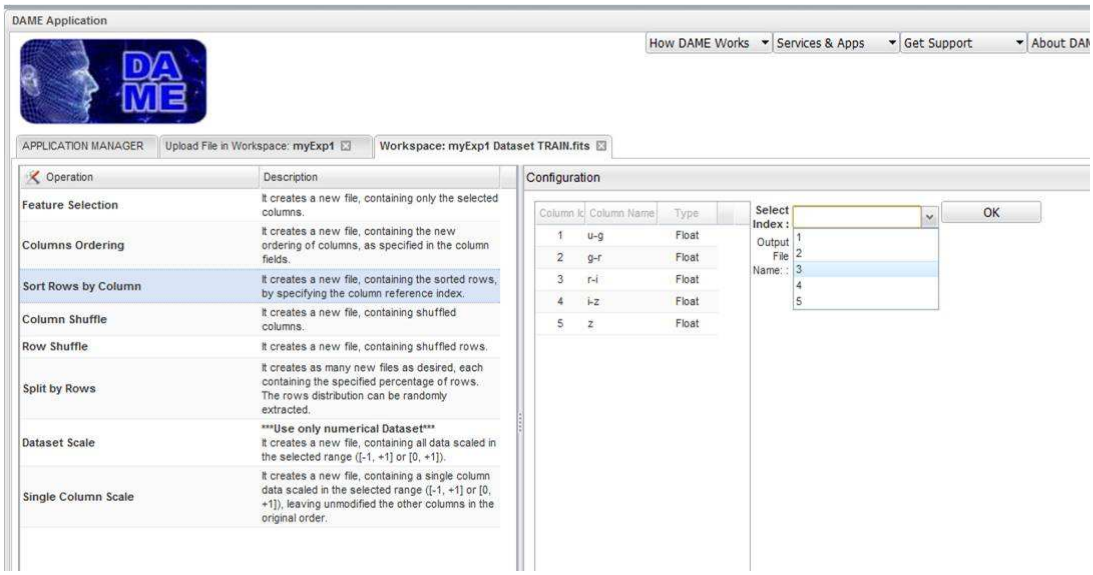

DAME Application
How DAME Works
Services & Apps
Get Support
About DAM
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Idx
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Select Index :
Output File Name: :
1
2
3
4
5
OK

Fig. 31 – The Sort Rows by Column operation – step 1

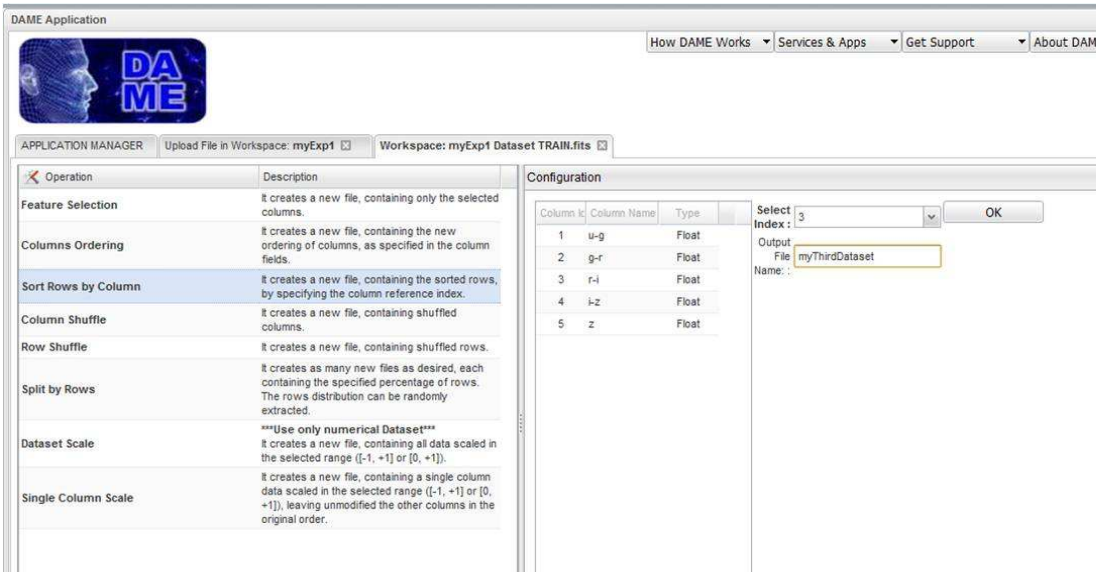

DAME Application
How DAME Works
Services & Apps
Get Support
About DAM
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Idx
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Select Index :
3
Output File Name: :
myThirdDataset
OK

Fig. 32 – The Sort Rows by Column operation – step 2

This document contains proprietary information of DAME project Board. All Rights Reserved.

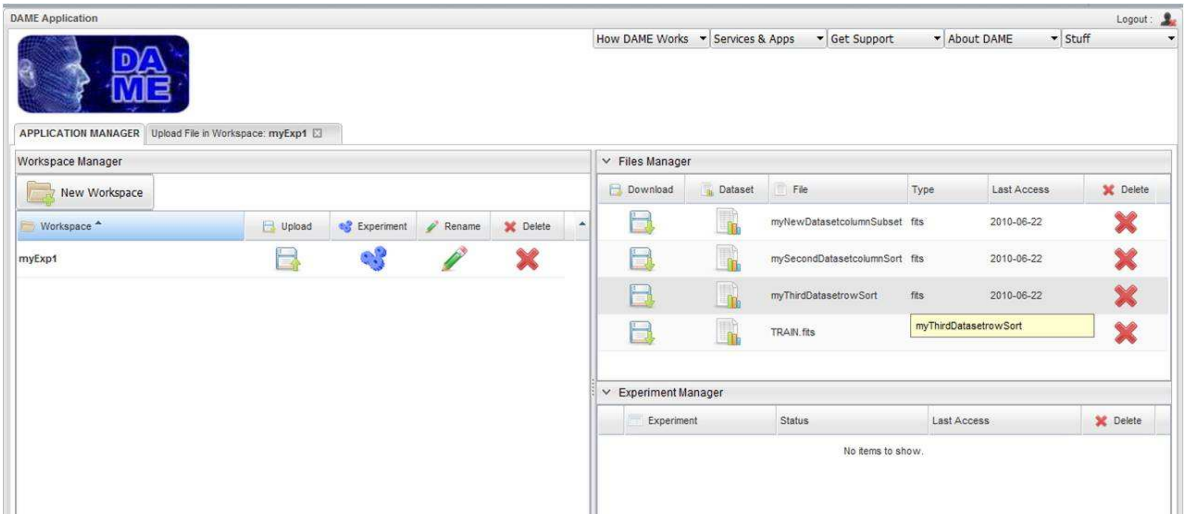


Fig. 33 – The Sort Rows by Column operation – the new file created

4.6.2.4 Column Shuffle

This dataset operation permits to operate a random shuffle of the columns, contained in the original data file. The result is the creation of a new file (of the same type and with the same extension of the original file), named as <user selected name>shuffle (i.e. with specific suffix *shuffle*). Details of the simple procedure are reported in Fig. 34 and Fig. 35.

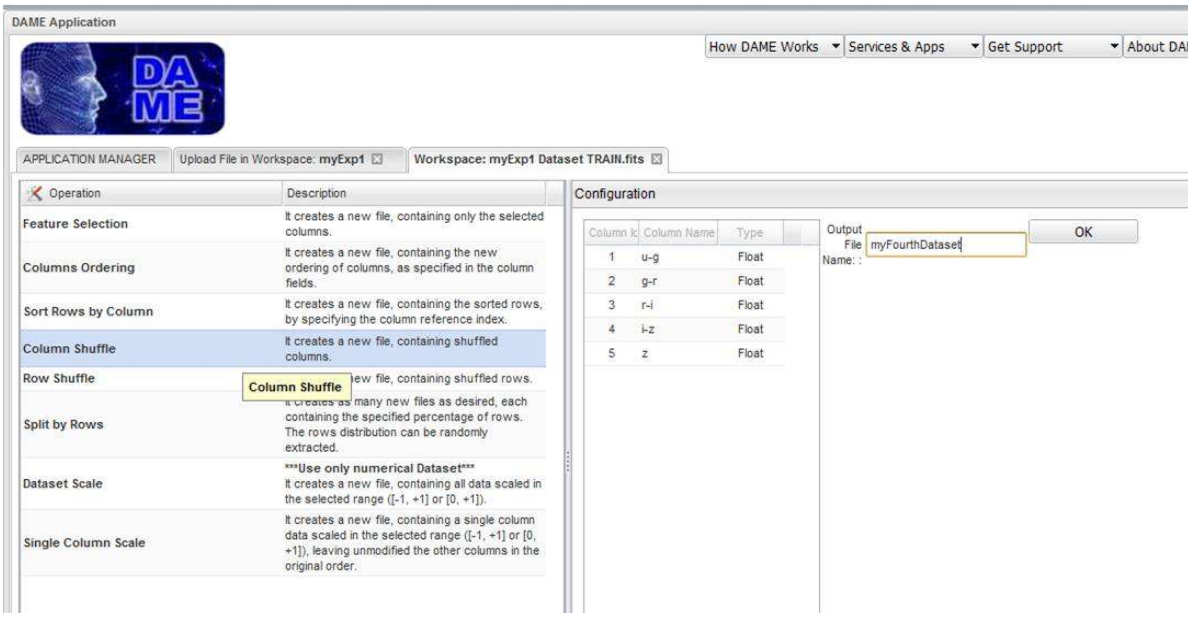

DAME Application
How DAME Works
Services & Apps
Get Support
About DA
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
Column Shuffle
Split by Rows
The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Output File Name:
myFourthDataset
OK

Fig. 34 – The Column Shuffle operation – step 1

This document contains proprietary information of DAME project Board. All Rights Reserved.

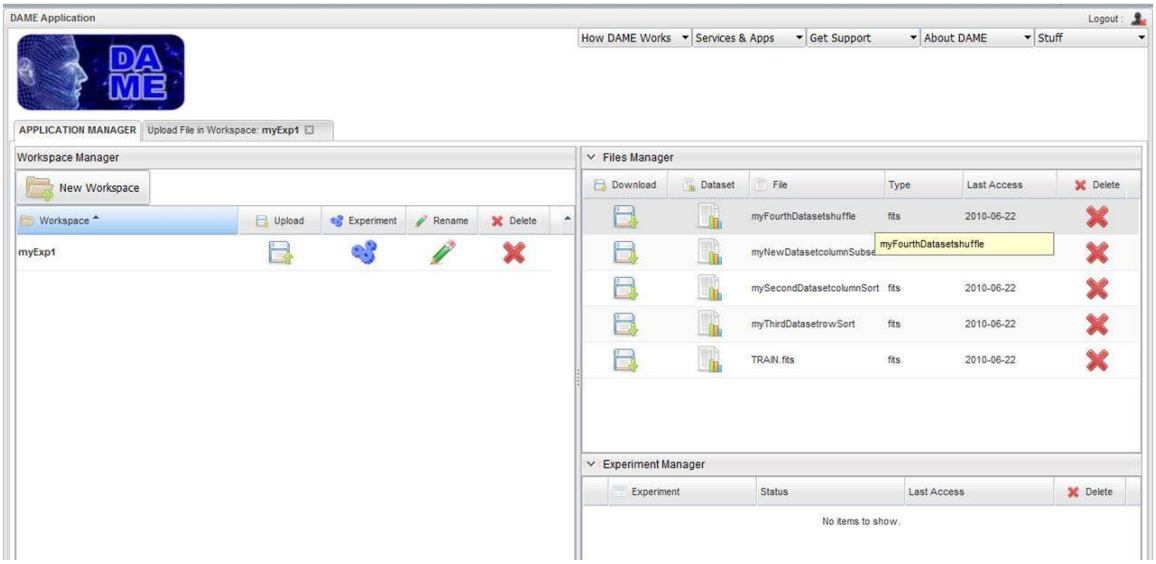


Fig. 35 – The Column Shuffle operation – the new file created

4.6.2.5 Row Shuffle

This dataset operation permits to operate a random shuffle of the rows, contained in the original data file. The result is the creation of a new file (of the same type and with the same extension of the original file), named as <user selected name>rowShuffle (i.e. with specific suffix *rowShuffle*). Details of the simple procedure are reported in Fig. 36 and Fig. 37.

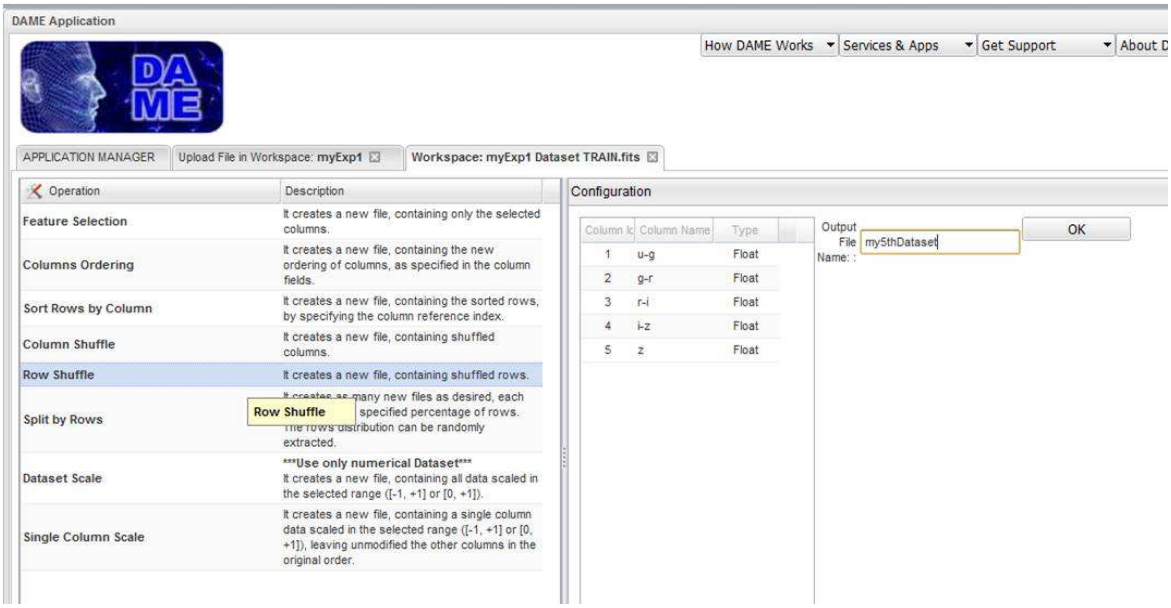

DAME Application
How DAME Works
Services & Apps
Get Support
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
Row Shuffle
specified percentage of rows.
The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Output File Name: :
my5thDataset
OK

Fig. 36 – The Row Shuffle operation – step 1

This document contains proprietary information of DAME project Board. All Rights Reserved.

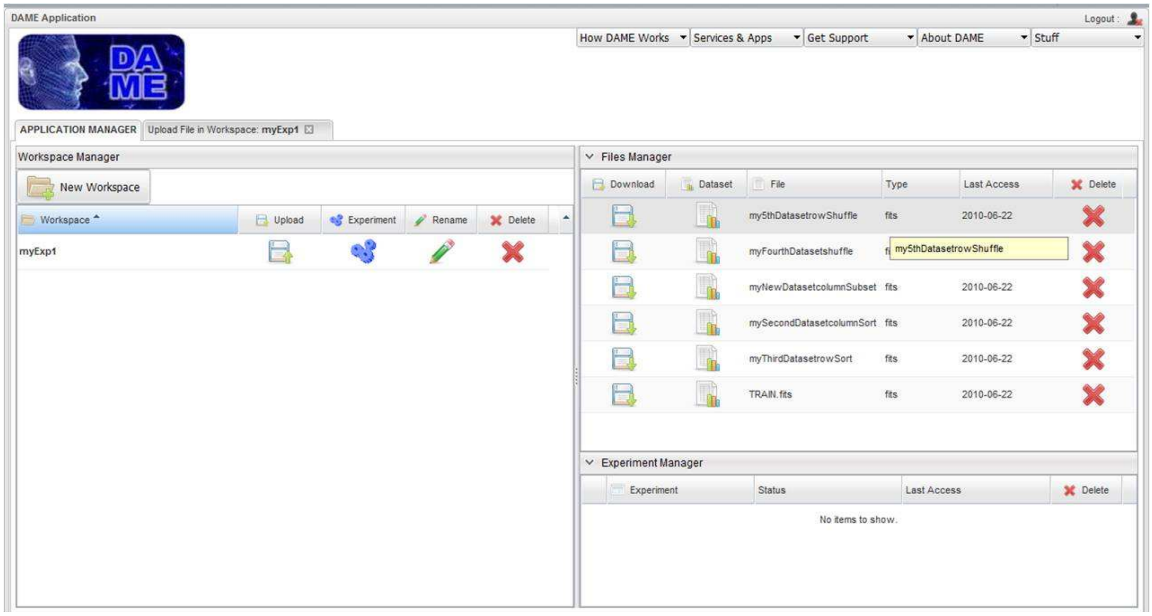


Fig. 37 – The Row Shuffle operation – the new file created

4.6.2.6 Split by Rows

This dataset operation permits to split the original file into two new files containing the selected percentages of rows, as indicated by the user. The user can move one of the two sliding bars in order to fix the desired percentage. The other sliding bar will automatically move in the right percentage position. The new file names are those filled in by the user in the proper name fields as <user selected name>_split1(_split2) (i.e. with specific suffix *split1*and *split2*). Details of the simple procedure are reported in Fig. 38, Fig. 39, Fig. 40.

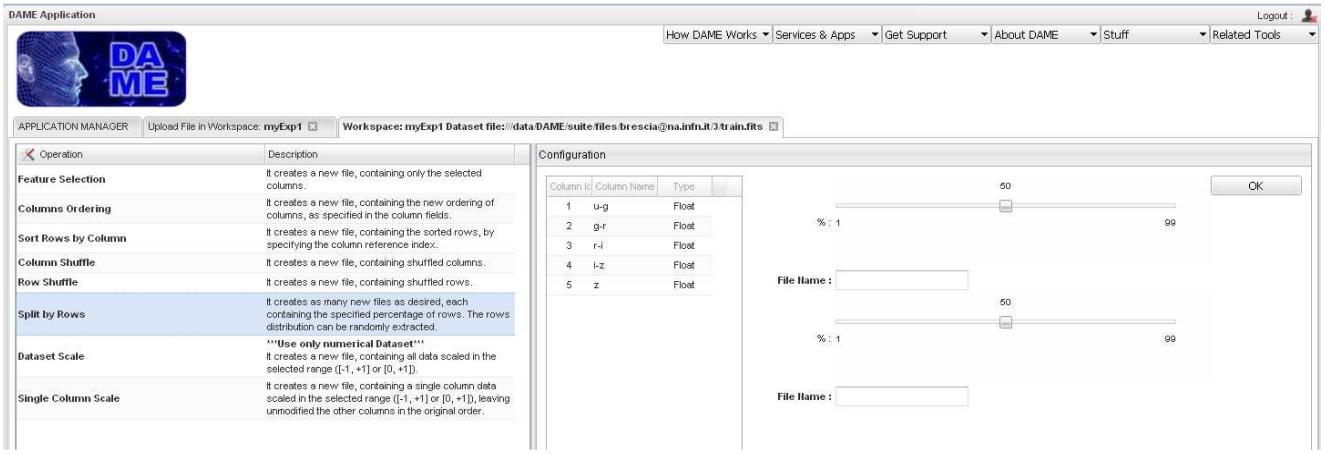

DAME Application
Logout :
How DAME Works
Services & Apps
Get Support
About DAME
Stuff
Related Tools
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset file:///data/DAME/suite/files/brescia@na.infn.it/3/train.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
'''Use only numerical Dataset'''
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
50
% : 1
99
OK
File Name :
50
% : 1
99
File Name :

Fig. 38 – The Split by Rows operation – step 1

This document contains proprietary information of DAME project Board. All Rights Reserved.

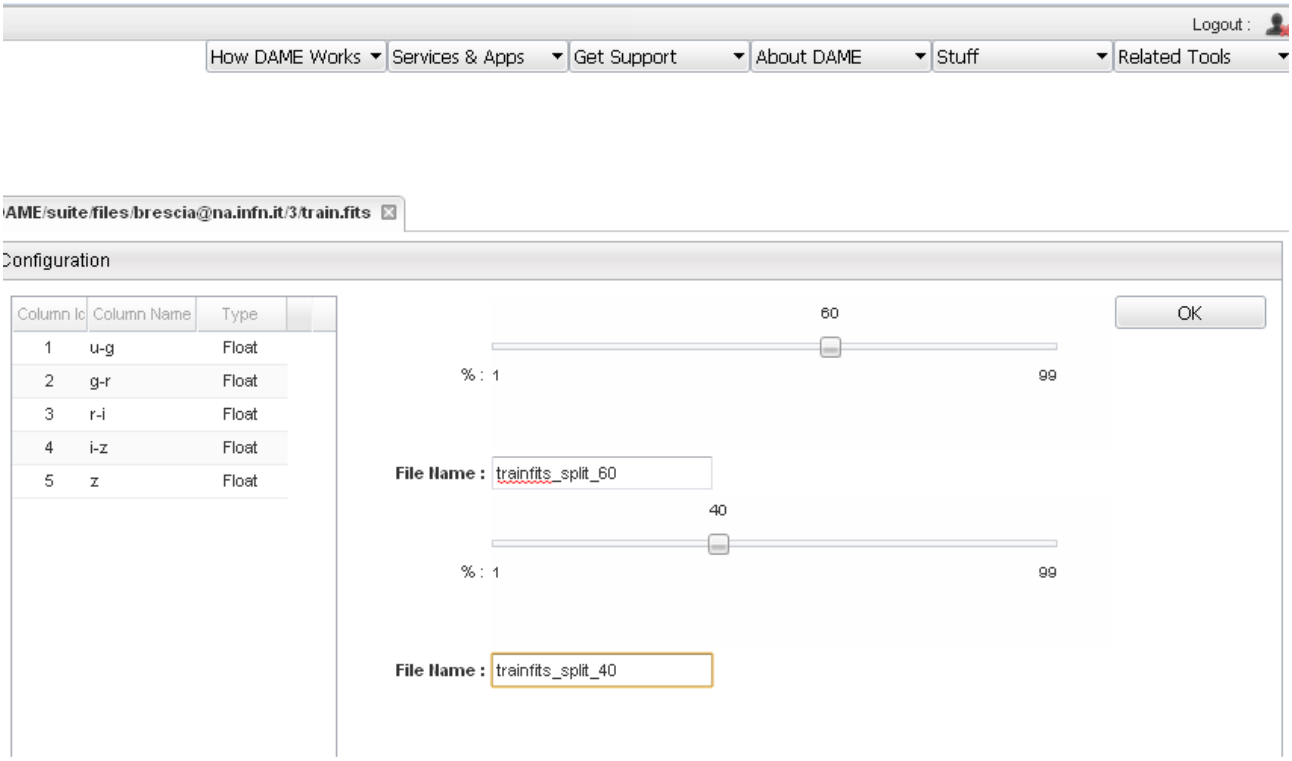


Fig. 39 – The Split by Rows operation – step 2

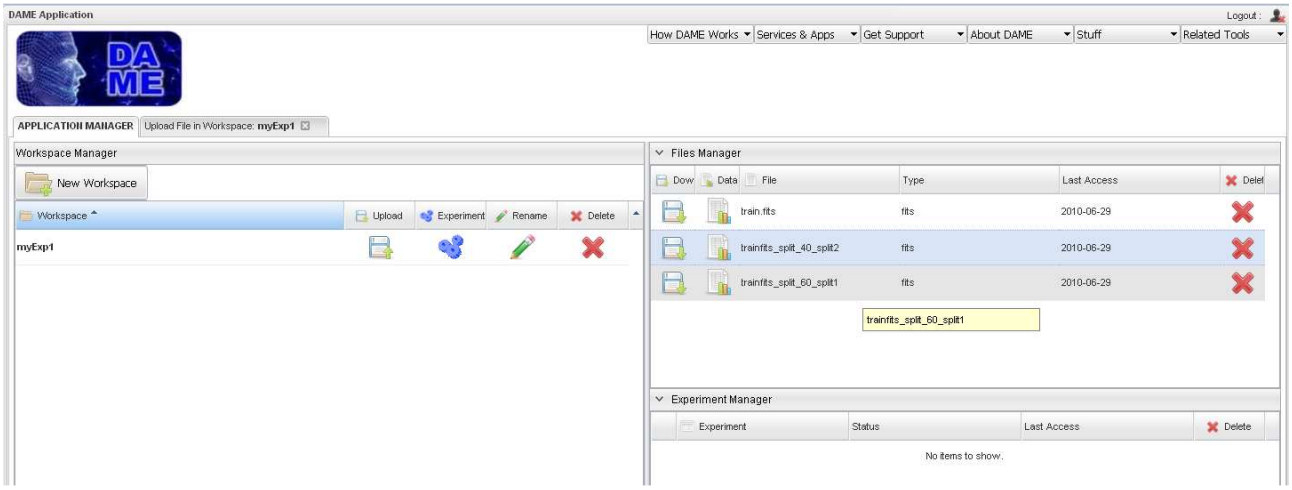


Fig. 40 – The Split by Rows operation – the new files created

4.6.2.7 Dataset Scale

This dataset operation (that works on numerical data files only!) permits to normalize column data in one of two possible ranges, respectively, [-1, +1] or [0, +1]. This is particularly frequent in machine learning experiments to submit normalized data, in order to achieve a correct training of internal patterns. The result is the creation of a new file (of the same type and with the same extension of the original file), named as

This document contains proprietary information of DAME project Board. All Rights Reserved.

<user selected name>scale (i.e. with specific suffix *scale*). Details of the simple procedure are reported in Fig. 41 and Fig. 42.

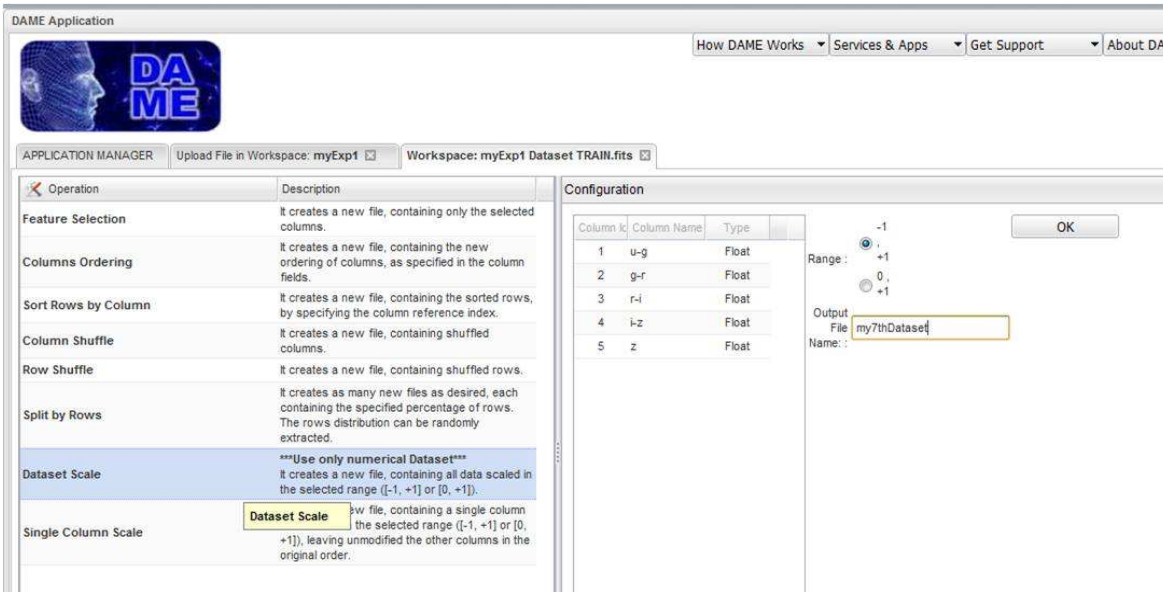

DAME Application
How DAME Works
Services & Apps
Get Support
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
Dataset Scale
Configuration
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
Range :
Output File Name: :
my7thDataset
OK

Fig. 41 – The Dataset Scale operation – step 1

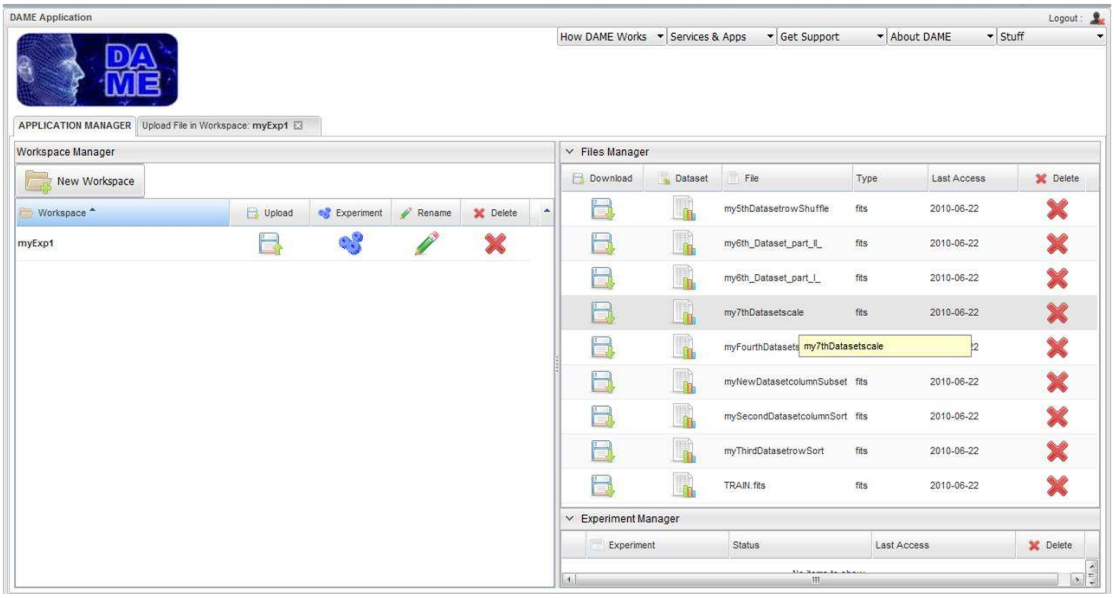


Fig. 42 – The Dataset Scale operation – the new file created

4.6.2.8 Single Column Scale

This dataset operation (that works on numerical data files only!) permits to normalize a single selected column, between those contained in the original file, in one of two possible ranges, respectively, [-1, +1] or [0, +1]. The result is the creation of a new file (of the same type and with the same extension of the original file), named as <user selected name>scaleOneCol (i.e. with specific suffix *scaleOneCol*). Details of the simple procedure are reported in Fig. 43, Fig. 44 and Fig. 45.

This document contains proprietary information of DAME project Board. All Rights Reserved.

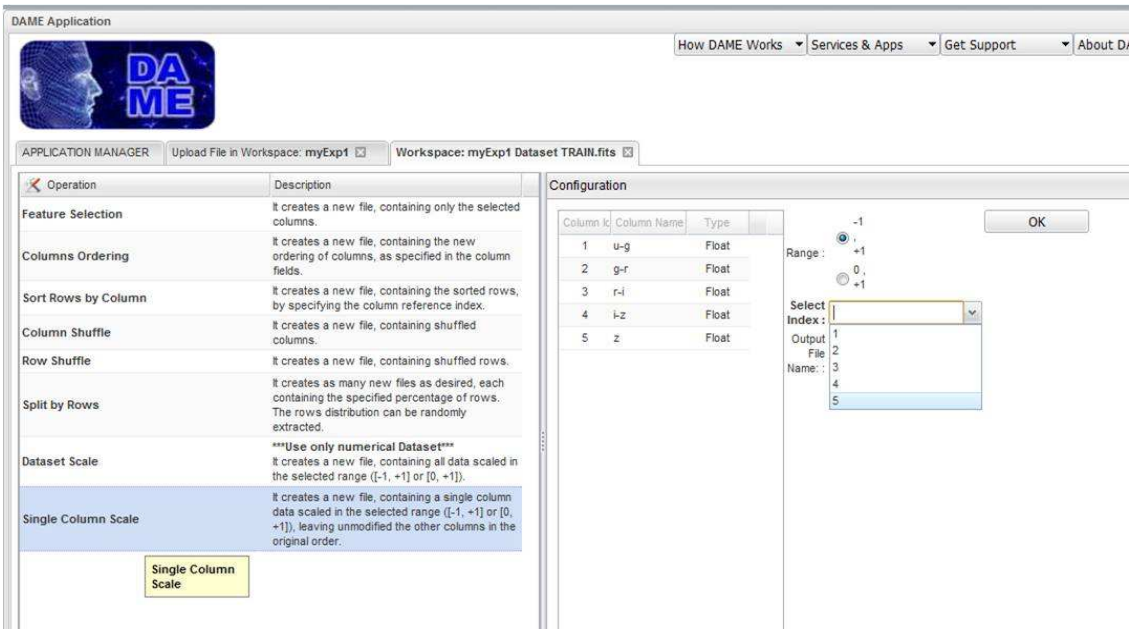

DAME Application
How DAME Works
Services & Apps
Get Support
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Single Column Scale
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
OK
Range :
Select Index :
Output File Name: :

Fig. 43 – The Single Column Scale operation – step 1

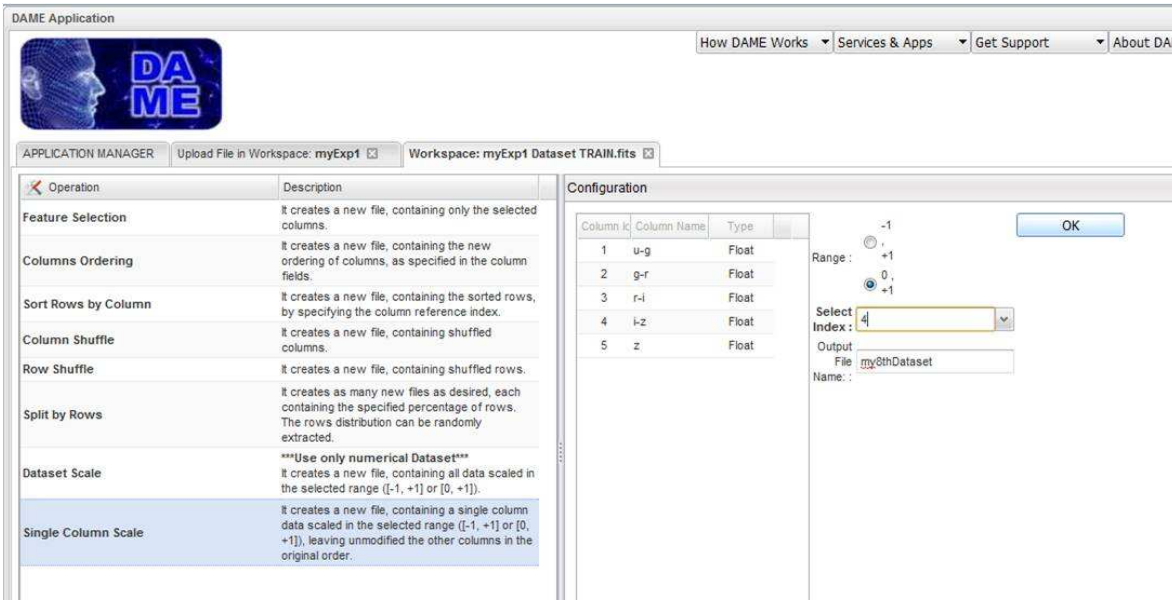

DAME Application
How DAME Works
Services & Apps
Get Support
APPLICATION MANAGER
Upload File in Workspace: myExp1
Workspace: myExp1 Dataset TRAIN.fits
Operation
Description
Feature Selection
It creates a new file, containing only the selected columns.
Columns Ordering
It creates a new file, containing the new ordering of columns, as specified in the column fields.
Sort Rows by Column
It creates a new file, containing the sorted rows, by specifying the column reference index.
Column Shuffle
It creates a new file, containing shuffled columns.
Row Shuffle
It creates a new file, containing shuffled rows.
Split by Rows
It creates as many new files as desired, each containing the specified percentage of rows. The rows distribution can be randomly extracted.
Dataset Scale
Use only numerical Dataset
It creates a new file, containing all data scaled in the selected range ([-1, +1] or [0, +1]).
Single Column Scale
It creates a new file, containing a single column data scaled in the selected range ([-1, +1] or [0, +1]), leaving unmodified the other columns in the original order.
Configuration
Column Id
Column Name
Type
1 u-g Float
2 g-r Float
3 r-i Float
4 i-z Float
5 z Float
OK
Range :
Select Index : 4
Output File Name: : my8thDataset

Fig. 44 – The Single Column Scale operation – step 2

This document contains proprietary information of DAME project Board. All Rights Reserved.

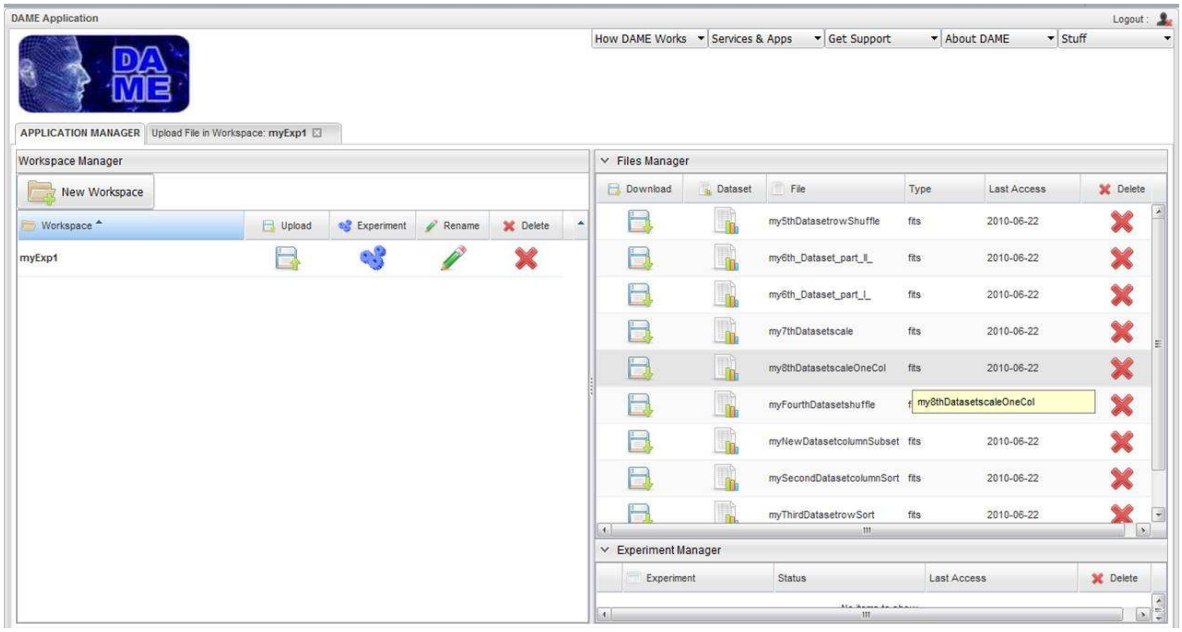


Fig. 45 – The Single Column Scale operation – the new file created

4.6.3 Download data

All data files (not only those of supported type) listed in the workspace and/or in the experiment panels, respectively, “Files Manager” and “Experiment Manager”, can be downloaded by the user on his own hard disk, by simply selecting the icon labelled with “Download” in the mentioned panels.

4.6.4 Moving data files

The virtual separation of user data files between workspace and experiment files, located in the respective panels (“Files Manager” for workspace files, and “Experiment Manager” for experiment files), is due to the different origin of such files and depends on their registration policy into the web application database. The data files present in the workspace list (“Files Manager” panel) are usually registered as “input” files, i.e. to be submitted as inputs for experiments. While others, present in the experiment list (“Experiment manager” panel), are considered as “output” files, i.e. generated by the web application after the execution of an experiment.
It is not rare, in machine learning complex workflows, to re-use some output files, obtained after training phase, as inputs of a test/validation phase of the same experiment. This is true for example for a MLP weight matrix file, output of the training phase, to be re-used as input weight matrix of a test (or validation) session of the same network.
In order to make available this fundamental feature in our application, the icon command nr. 14 in Fig. 14, associated to each output file of an experiment, can be selected by the user in order to “move” the file from experiment output list to the workspace input list, becoming available as input file for new experiments belonging to the same workspace[11]. As an example see Fig. 55.

[11] In the Alpha release it is forbidden to exchange files between experiments or between workspaces, but only from an experiment file list to the related workspace file list. So far, if the user wants to use the same data file for two different experiments, created into different workspaces, the multiple uploading of the same file is required.

This document contains proprietary information of DAME project Board. All Rights Reserved.

4.7 Experiment Management

After creating at least one workspace, populating it with input data files (of supported type) and optionally creating any dataset file, the next logical operation required is the configuration and launch of an experiment. The Fig. 46 shows the initial step required, i.e. the selection of the icon command nr. 6 of Fig. 14 in order to name the new experiment.

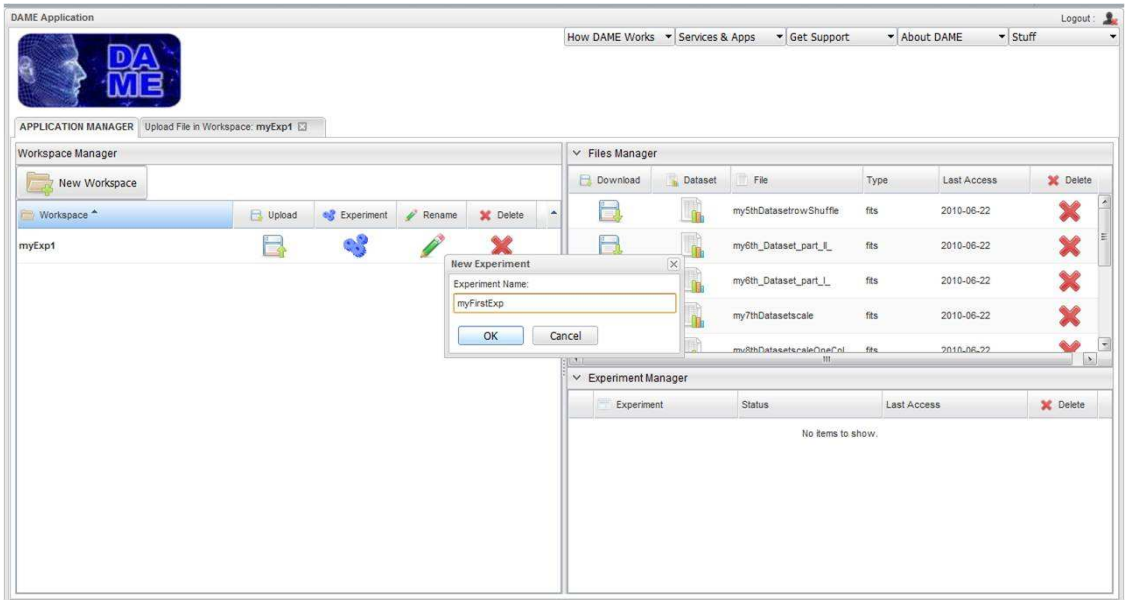


Fig. 46 – Creating a new experiment (by selecting icon "Experiment" in the workspace)

Immediately after, an automatic new tab appears, making available all basic features to select, configure and launch the experiment, Fig. 47.

The following is the complete list of all parameters that the user can set with MLP. Their quantity and typology depends on which use case is selected for the experiment;

- **Network File**: this field should be used only when the user wants to re-use an already trained internal weight matrix for the MLP. If empty, a random initial weight matrix for hidden nodes is generated;
- **Number of input nodes**: the input nodes must match the number of input columns as included in the dataset currently used. It must be maintained unchanged in all use cases related with the same experiment;
- **Number of nodes for hidden layer**: this field specifies the number of internal nodes composing the hidden layer of MLP. There are no magic numbers for this field. It basically depends on the complexity of your experiment (see section 3.3.1.3.3).
- **Number of output nodes**: this number must match the number of "target" columns of the user dataset, and it must be maintained unchanged in all use cases related with the same experiment;
- **Number of iterations**: this is one of the stopping criteria of the algorithm. A small number could speed up the training duration but limiting the convergence to the learning minimum error threshold;
- **error tolerance**: this is the second stopping criterion of the algorithm. This is the minimum error threshold for the convergence of the learning method. It should be very small in order to operate a maximum refinement of the training;

This document contains proprietary information of DAME project Board. All Rights Reserved.

- **training mode**: this is a very important parameter. It deals with the strategy adopted in the algorithm to submit input patterns, together with the criterion used to evaluate the network output in terms of function applied to the comparison between network outputs and targets. The basics about these options is described in section 3.3.1.4. Here we remark that the choice for this parameter depends on which functionality has been selected;
    - **In case of Regression**: two different choices are available:
        - (MSE+batch);
        - (MSE+incremental);
    - **In case of Classification**:
        - (MSE+batch);
        - (MSE+incremental);
        - (CE+batch);
        - (CE+incremental);

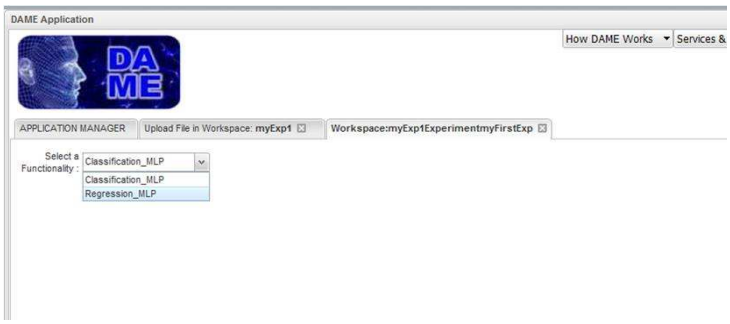


Fig. 47 – The new tab reporting the list of functionality-model couples available for experiments

In the alpha release, the only two options available for experiment are Classification with MLP and Regression with MLP. The user should select the couple that better matches with the desired experiment type is going to do.

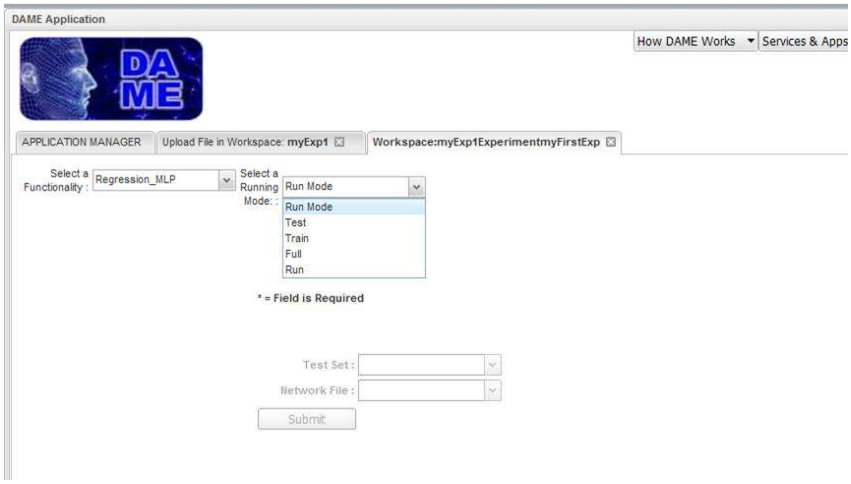


Fig. 48 – The use case selection for the experiment

This document contains proprietary information of DAME project Board. All Rights Reserved.

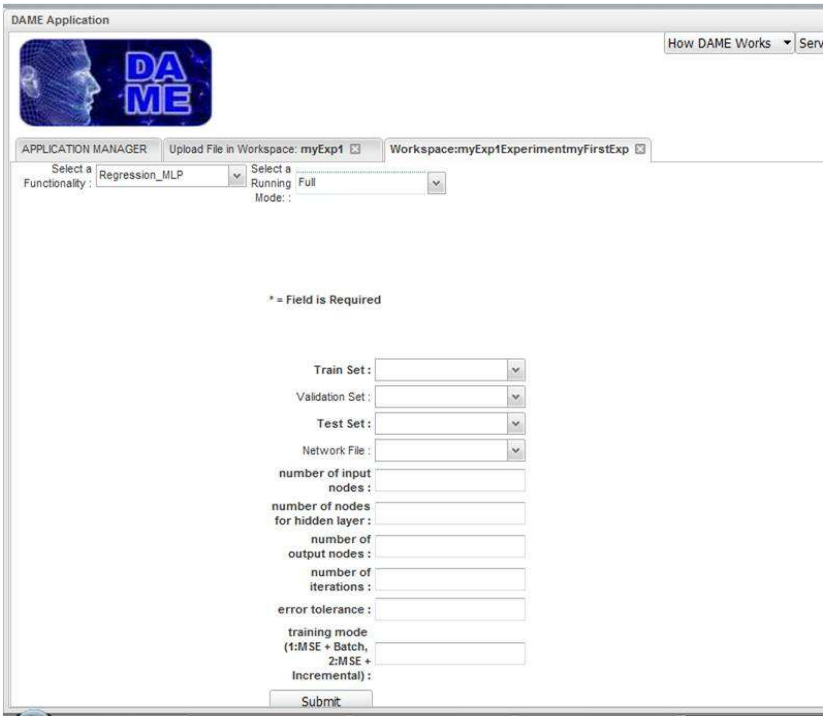


Fig. 49 – The experiment parameter list for the use case "Full" in the regression case

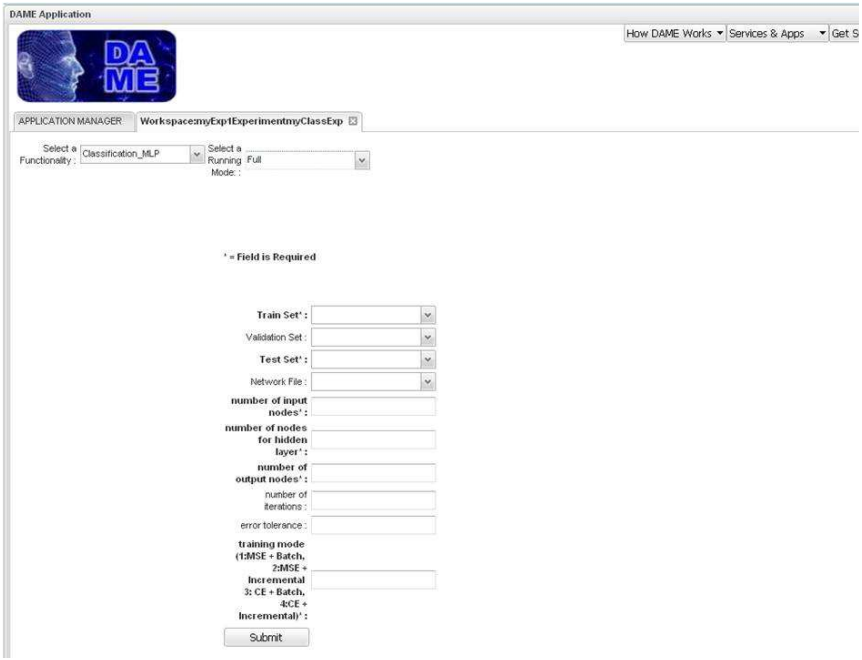


Fig. 50 – The experiment parameter list for the use case "Full" in the classification case

This document contains proprietary information of DAME project Board. All Rights Reserved.

Fig. 51 – The experiment parameter list for the use case "Train"

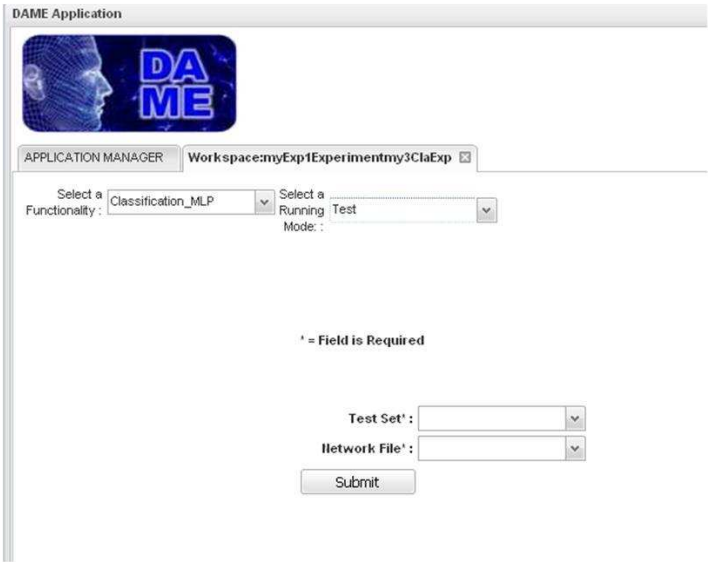


Fig. 52 – The experiment parameter list for the use case "Test"

This document contains proprietary information of DAME project Board. All Rights Reserved.

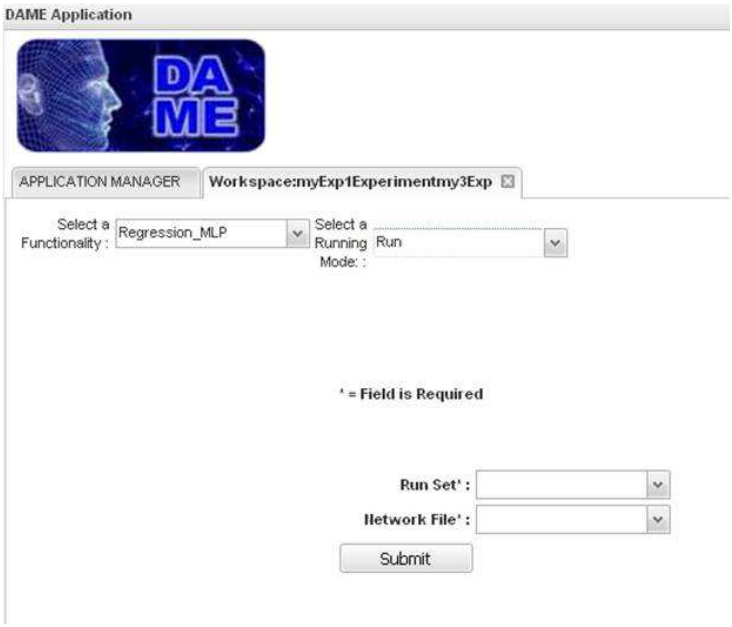


Fig. 53 – The experiment parameter list for the use case "Run"

Any experiment can be result in one of the following states (example in Fig. 54):

- **Enqueued**: if the multi-thread processing system results busy, the execution is put in the job queue;
- **Running**: the experiment has been launched and it is running;
- **Failed**: the experiment has been stopped or concluded and any error occurred;
- **Ended**: the experiment has been successfully concluded;

Fig. 54 – Some different state of two concurrent experiments

4.7.1 Re-use of already trained networks

In the previous section a general description of experiment use cases has been reported. A specific more detailed information is required by the "Run" use case. As known this is the use case selected when a network (in the alpha release case an MLP) has been already trained (i.e. after training use case already executed). The Run case is hence executed to perform scientific experiments on new data. Remember also that the input file does not include "target" values. The execution of a Run use case, for its nature, requires special steps in the DAME Suite. These are described in the following.

As first step, we require to have already performed a train case for any experiment, obtaining a list of output files (train or full use cases already executed). In particular in the output list of the train/full experiment there

This document contains proprietary information of DAME project Board. All Rights Reserved.

is the file *outputFileName_netTrain.mlp*, as remarked in section 3.3.1.4. This file contains the final trained network, in terms of final updated weights of neuron layers, exactly as resulted at the end of the training phase. Depending on the training correctness this file has in practice to be submitted to the network as initial weight file, in order to perform running sessions on input data (without target values).

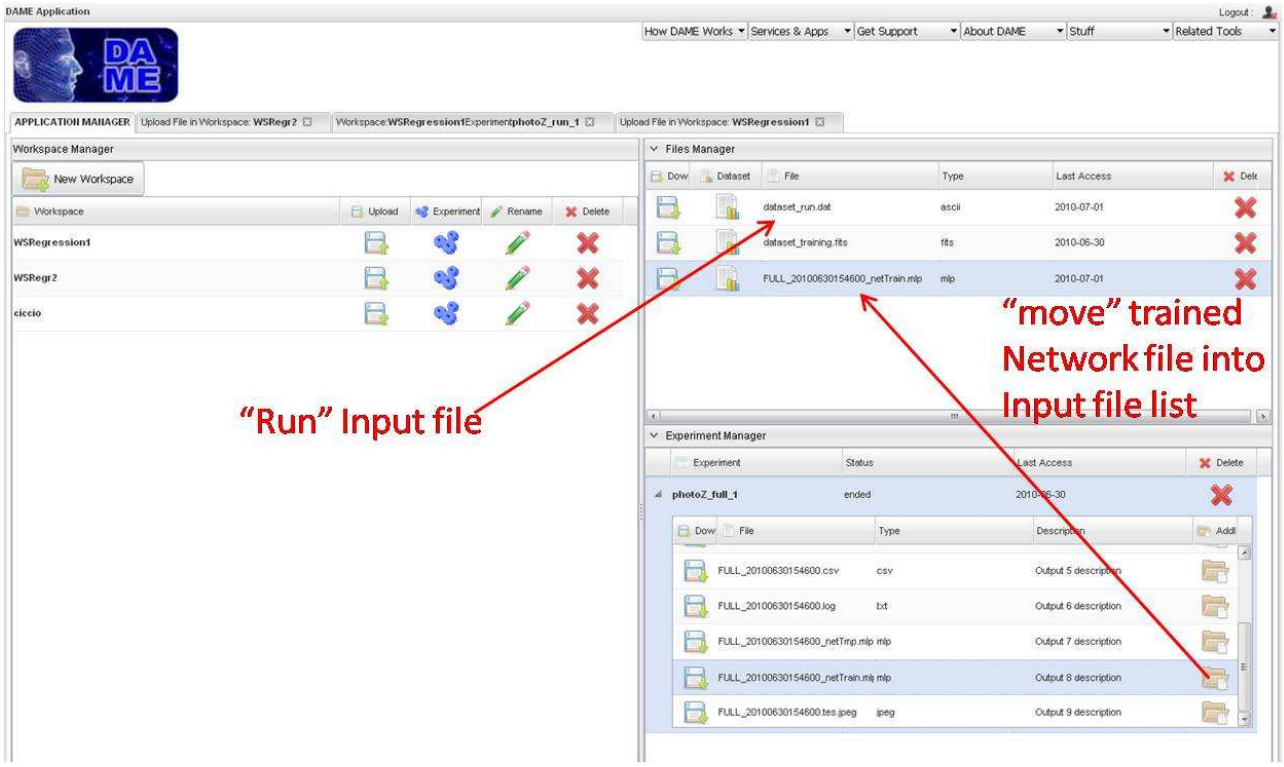


Fig. 55 – The operation to "move" an output file in the Workspace input file list

To do this, the output weight file must become an input file in the workspace file list, as already explained in section 4.6.4, otherwise it cannot be used as input of Run use case experiment, Fig. 55. Also, the workspace currently active, hosting the experiment we are going to do, must contain a proper input file for Run cases, i.e. without target columns inside.
So far, the second step is to populate the workspace file list with trained network and Run compliant input files, as shown in Fig. 55, where experiment "photoZ_full_1" is the training experiment, already concluded, and its network file *.mlp* we want to use as network trained weight file for future Run experiments.

This document contains proprietary information of DAME project Board. All Rights Reserved.

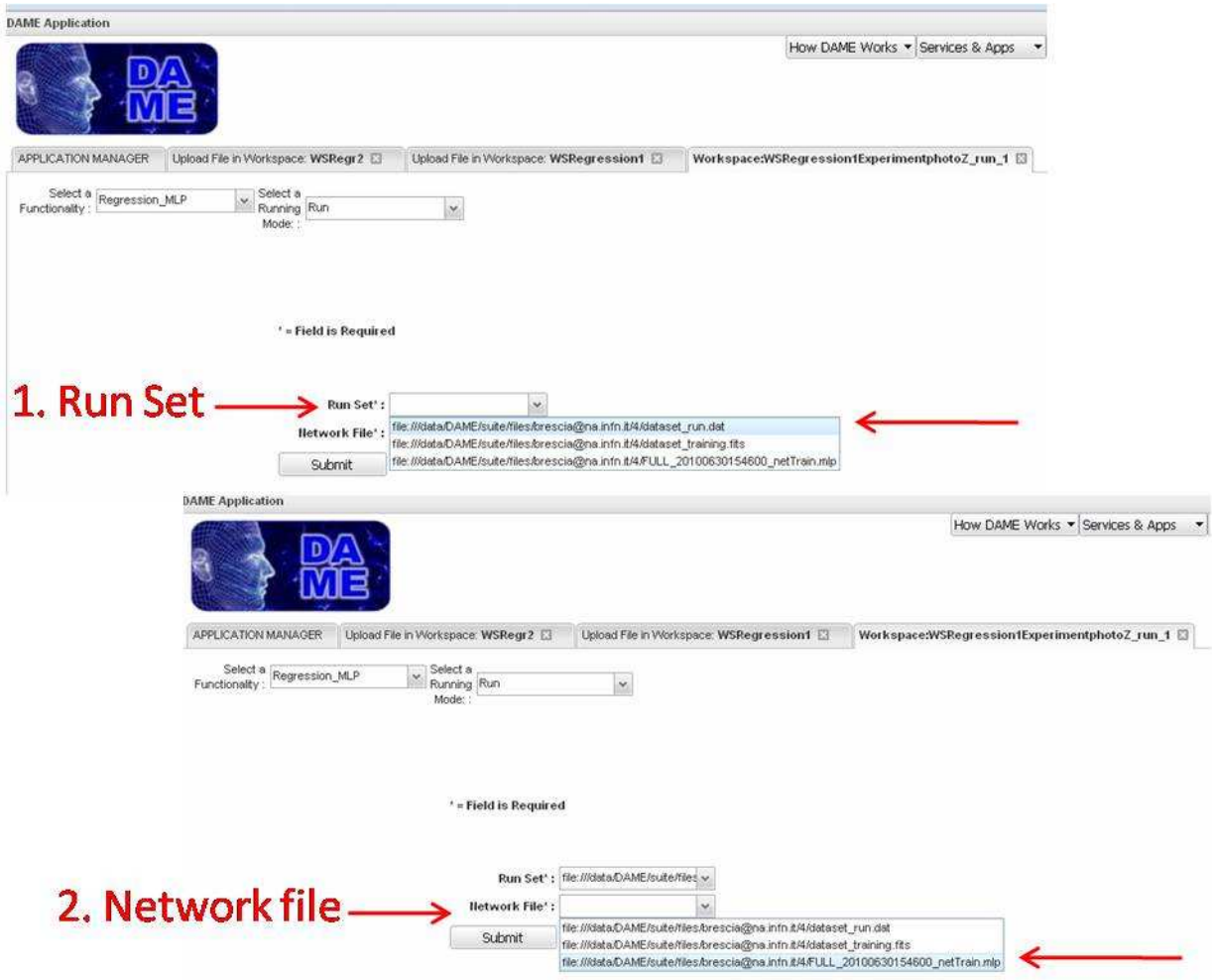


Fig. 56 – The choice of input parameters of Run use case experiment

After that, the third step is to create a new experiment in the current workspace (i.e. the same hosting the already done training experiment) and to configure its parameters. These are basically two: the Run data input file (one present in the workspace without target columns inside) and the network weight file (output of the previous train/full use case experiment). After selecting these two parameters the Run experiment can be launched, Fig. 56.

This document contains proprietary information of DAME project Board. All Rights Reserved.

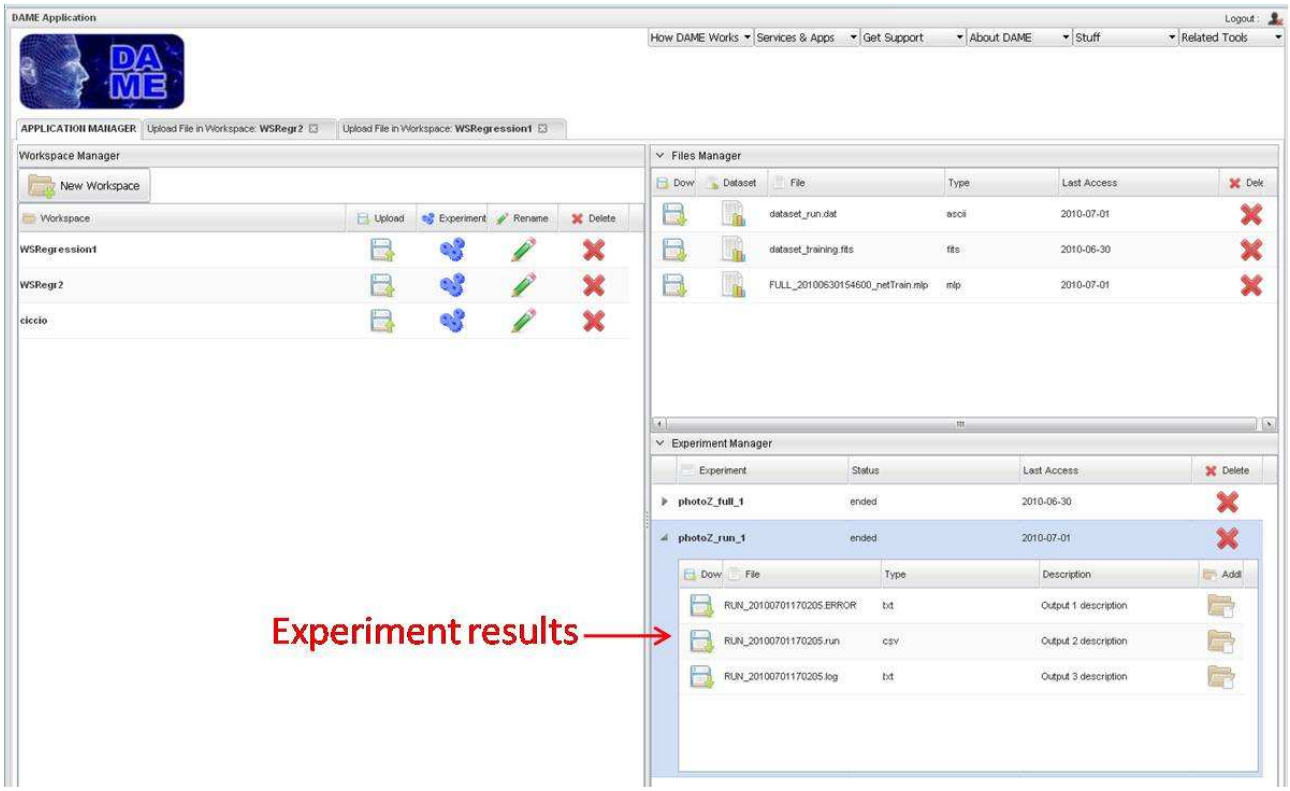


Fig. 57 – Some different state of two concurrent experiments

At the end of Run experiment execution, the experiment output area should contain a list of output files, as shown in Fig. 57.

Also the same file *outputFileName_netTrain.mlp* should be selected as Network file input in case you want to execute another training (TRAIN/FULL cases) phase, for example when first training session ended in an unsuccessful or insufficient way. In this cases the user can execute more training experiments, starting learning from the previous one, by resuming the trained weight matrix as input network for future training sessions.. This operation is the so-called "*resume training*" phase of a neural network.

This document contains proprietary information of DAME project Board. All Rights Reserved.

5 A practical example

The best way to make clear the scientific use of the DM Suite features, we invite the reader to follow the example described here. In what follows we will train the MLP model to perform a regression problem.

5.1.1 The scientific problem: Photometric redshifts estimation

Photometric redshifts have become one of the main tools to investigate the spatial distribution of galaxies, since they are necessary to reconstruct the 3-dimensional position of very large number of sources using only their photometric properties. The mechanism responsible of the correlation between the photometric features and the redshift of an astronomical source, is the change in the contribution to the observed fluxes caused by the prominent features of the observed spectrum continuum and line emission components shifting through the different filters of the photometric system as the spectrum of the source is redshifted, [R5].
One family of methods for photometric redshift estimation is called "empirical" since these methods can be applied only to "mixed surveys", i.e. to datasets where accurate multiband photometric observations for a large number of source are supplemented by spectroscopic redshifts for a smaller but still significant subsample of the same sources, representative from a statistical point of view of the parent population. These spectroscopic data are used to constrain the fit of an interpolating function mapping the photometric parameter space; different specific methods differ mainly in the way such interpolation is performed. Neural networks (NN), among other machine learning algorithms, are very efficient at recognizing relations between data and in the "training phase" they need a set of "examples" to learn efficiently how to reconstruct the relation between the "parameters" and the "target". In the specific case of photometric redshifts, the parameters are fluxes, magnitudes or colours of the extragalactic sources while the targets, an independent and reliable estimate of the quantity the NN are trained to evaluate, are the redshifts of the sources measured from their observed spectra.
In other words, multicolor photometry maps physical parameters (luminosity L, redshift z and spectral type T) into observed fluxes. If this relation can be inverted it could be possible to estimate the parameters (in particular the redshift z) from information about magnitudes or colors of extragalactic sources. So far, the inverted function can be approximated by regression in the photometric space.

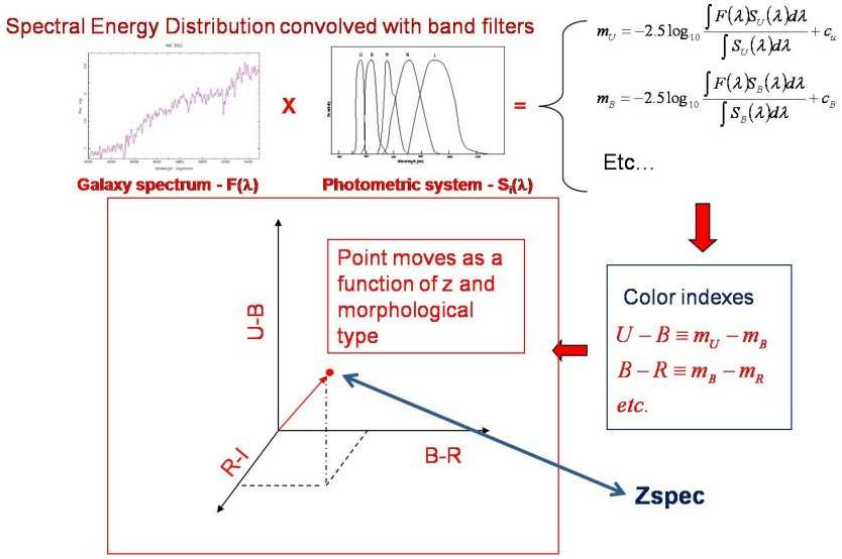


Fig. 58 – The relation between redshift, color and source observed fluxes

This document contains proprietary information of DAME project Board. All Rights Reserved.

Starting from a sample of SDSS galaxy population, where spectroscopic redshifts zspec are known, we want to train a MLP to learn correlation between color indexes (or magnitudes) and zspec, in order to be able to estimate, after training, the corresponding photometric redshifts zphot for all sources (not only those used for the training; this feature is defined as "generalization" in the neural network discipline).
The main considerations about the effectiveness of such scientific experiment are:

- Spectroscopic observations are the most accurate method to determine redshifts, but time consuming;
- Photometric sources often outnumber Spectroscopic ones up to 3 orders of magnitude (it may depend on the BoK);
- If we build a reliable BoK with spectroscopic data, we can reproduce the functional mapping between photometric parameters and redshift;
- zphot accuracy is adequate for several astronomical applications

5.1.2 The Base of Knowledge (BoK)

The BoK for this experiment is basically a data file[12] named train.fits, a FITS file containing 5 columns, respectively, first 4 columns with galaxy observed color indexes and last one reporting the zspec. For simplicity, in Fig. 59 the corresponding first rows of the ASCII version of the same file (train.dat) are reported (note that last column "z" is the zspec target column).

# u-g	g-r	r-i	i-z	z
1.732126	0.9546661	0.36711693	0.3048267	0.1100841
1.478172	0.8132877	0.40897083	0.3313818	0.0574778
1.703563	0.9014311	0.37031174	0.2970972	0.0934919
2.057241	0.9832868	0.38784504	0.2870807	0.0838121
1.746034	0.8216390	0.32788754	0.2738428	0.0303944
1.873275	0.9449444	0.36474895	0.3270979	0.0878967
1.379293	0.8810863	0.37609863	0.2776117	0.1327481
1.057239	1.7806321	0.52259636	0.3879566	0.3630241
1.506830	0.8800335	0.39445114	0.2670669	0.0851713
1.784950	0.8973875	0.35031796	0.3235330	0.0712303
1.673229	0.8538627	0.35259247	0.2430534	0.0850956
1.999797	1.0083599	0.40515518	0.2955246	0.0838573
1.926775	1.1577051	0.41964151	0.3187046	0.1568491

Fig. 59 – The 5 columns and first 13 rows of train.dat input file

As an alternative to train.fits, it is also possible to use the file dataset_train.fits (or the corresponding ASCII format, dataset_training.dat), composed by the same columns of train.fits but with a largest number of input patterns (rows).
Anyway for both files their natural use is related as training files for the network, because they contain first 4 "input" columns plus the "target" column, i.e. the correct output values associated with inputs.
Other files can be used for run the network after training phase. For example the file test.dat contains the same first 4 columns of train.dat, with the last "target" column missing. The "run" use case in fact, is performed to evaluate the generalization capability of the trained network, without giving as input the corresponding "target" values of the original BoK.
So far, remember that the MLP-BP model is a supervised type and all experiments require to train and test the network with couples "input" + "target" extracted from the available BoK for the experiment, using "input" values only in the run phase.

[12] Available at http://voneural.na.infn.it/alpha_info.html

This document contains proprietary information of DAME project Board. All Rights Reserved.

Intermediate phases, like test and validation use cases, are optional cases in which the user can submit a specific dataset (or in principle the same training dataset) with inputs+targets couples to respectively, test and validate the performances (see section 3.2.1.2 for details about validation techniques).

5.1.3 Dataset Manipulation

In case of desired variations in the present example, for example by inverting or excluding input columns or rows, the user should use the dataset editor features to create new modified input files for training, test and run experiments (see section 4.6.2 for details).
This kind of experiment variation is also strongly suggested, but when the user will have acquired a sufficient practice in the experiment setup and execution. This in order to evaluate the different degree of learning features of the same network model, strongly depending on the BoK used for training.

5.1.4 Experiment execution

Having supposed to be ready with the datasets, it is now time to start the experiment.

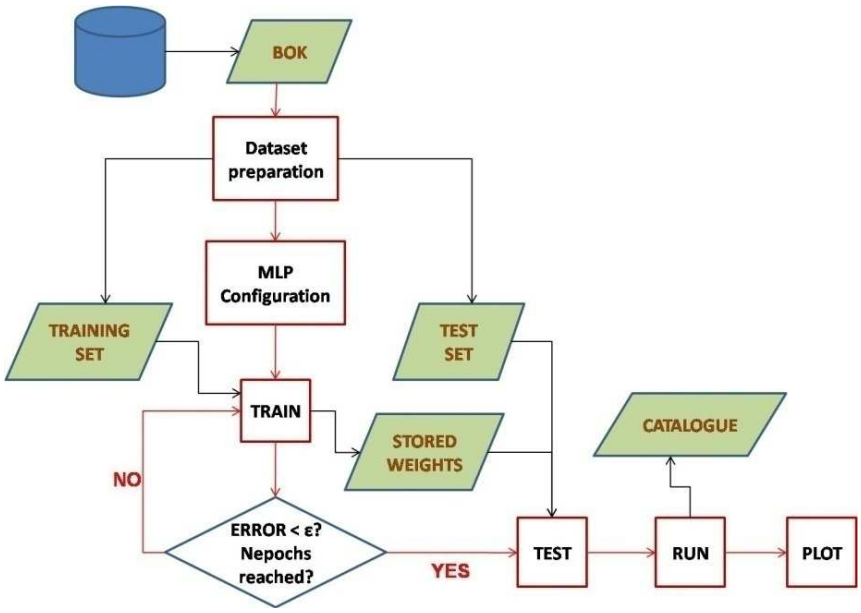


Fig. 60 – The complete flow-chart of the experiment with MLP model

The Fig. 60 shows the complete flow-chart of a generic experiment involving the MLP model. As described in the section 4.7, a complete MLP experiment requires a sequence of use cases, starting from training up to run case.
By following the rules issued in the mentioned section, it is also possible, for simplicity, configure and execute all the use cases in one shot, by selecting “full” use case in the experiment configuration tab. This is the case we will follow in this example.
So far, create a new experiment, called “myFirstExp”, as in Fig. 46, and open the experiment tab by selecting “Regression_MLP” as shown in Fig. 47.
Next step is the selection of the use case to be executed. In the example the “Full” use case is our choice. It is then necessary to fill in all experiment and model parameters.

This document contains proprietary information of DAME project Board. All Rights Reserved.

For simplicity in the present example we will exclude validation case and re-use the same dataset (e.g. train.fits) in both training and test cases, (see Fig. 61 and Fig. 62). But remember that usually different dataset would be used instead.

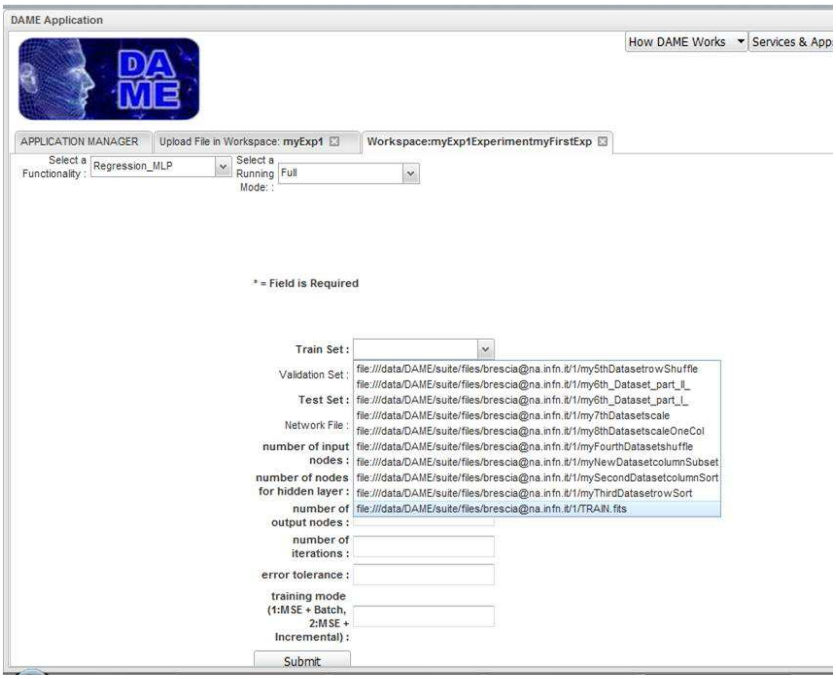


Fig. 61 – The selection of train.fits as Train Set

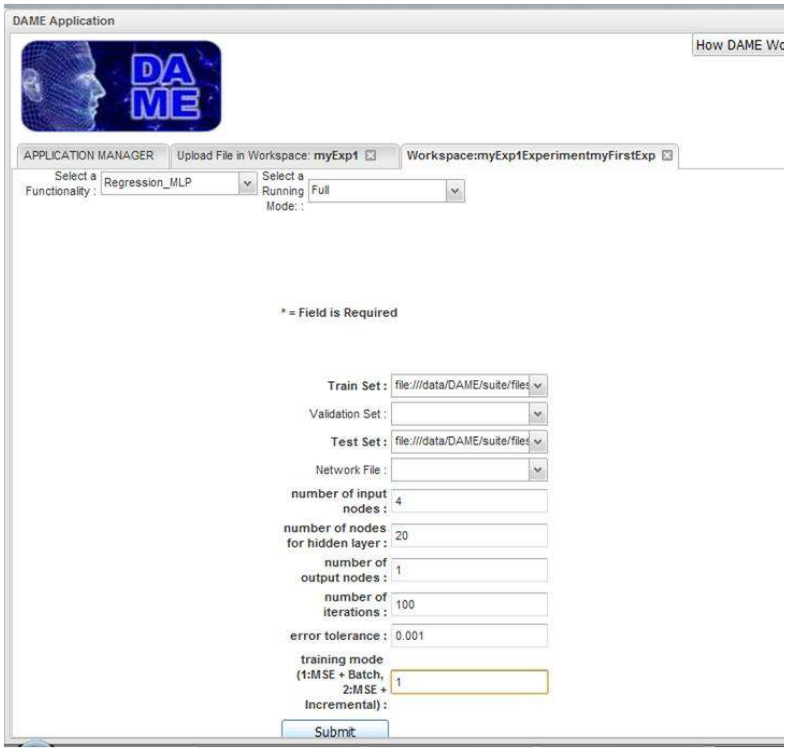


Fig. 62 – The selection of train.fits as Test Set and all fields compiled

This document contains proprietary information of DAME project Board. All Rights Reserved.

After the selection of datasets for train and test phases, we proceed to fill in other parameters, Fig. 62:

- **Network File**: this field is leaved empty (it should be used only when the user wants to re-use an already trained internal weight matrix for the MLP). If empty a random initial weight matrix for hidden nodes is generated;
- **Number of input nodes**: 4. Remember that the input nodes must match the number of input columns as included in the dataset currently used;
- **Number of nodes for hidden layer**: 20. This field specifies the number of internal nodes composing the hidden layer of MLP. There are no magic numbers for this field. It basically depends on the complexity of your experiment (see section 3.3.1.3.3).
- **Number of output nodes**: 1. Remember that this number depends on the number of "target" columns of the user dataset;
- **Number of iterations**: 100. Remember that this is one of the stopping criteria of the algorithm. A small number could speed up the training duration but limiting the convergence to the learning minimum error threshold;
- **error tolerance**: 0.001. This is the second stopping criterion of the algorithm. This is the minimum error threshold for the convergence of the learning method. It should be very small in order to operate a maximum refinement of the training;
- **training mode**: 1 (MSE+batch). In this case at each learning iteration all dataset training patterns are submitted to the network, and the weight adjustment is done at the end of the whole pattern presentation. The other method (MSE+incremental) is used when user wants to adjust weights after each single pattern calculation;

An interesting investigation, suggested to the user after having a sufficient practice with the model, could be to repeat same experiment by varying some of the above parameters, in order to evaluate results in terms of quality of zphot calculated, training error and convergence speed etc. This is one of the best heuristic methods to acquire experience with such methods.

5.1.5 Experiment Results

The DM Suite gives the possibility to list the output files at the end of the experiment execution. In the Regression_MLP experiment example the most important output files generated are the following, Fig. 63:

- Full.log: log file reporting the status of the last execution phase of the experiment, Fig. 64;
- Full.tra: ASCII file reporting two columns, respectively, network training output and corresponding target value, for each pattern (row), Fig. 65 - left;
- Full.tes: ASCII file reporting two columns, respectively, network test output and corresponding target value, for each pattern (row), Fig. 65 – right. Note that it corresponds to the Full.tra, because in the example the same dataset has been used for training and test phases;
- Full.csv: CSV file reporting the training error for each learning iteration, Fig. 66;
- Full.tes.jpeg: diagram reporting the graphical view of file Full.tes, Fig. 67;
- Full.csv.jpeg: diagram reporting the graphical view of file Full.csv, Fig. 68;

Depending on the use case and on the functionality-model chosen for the experiment, the output files may be different.

This document contains proprietary information of DAME project Board. All Rights Reserved.

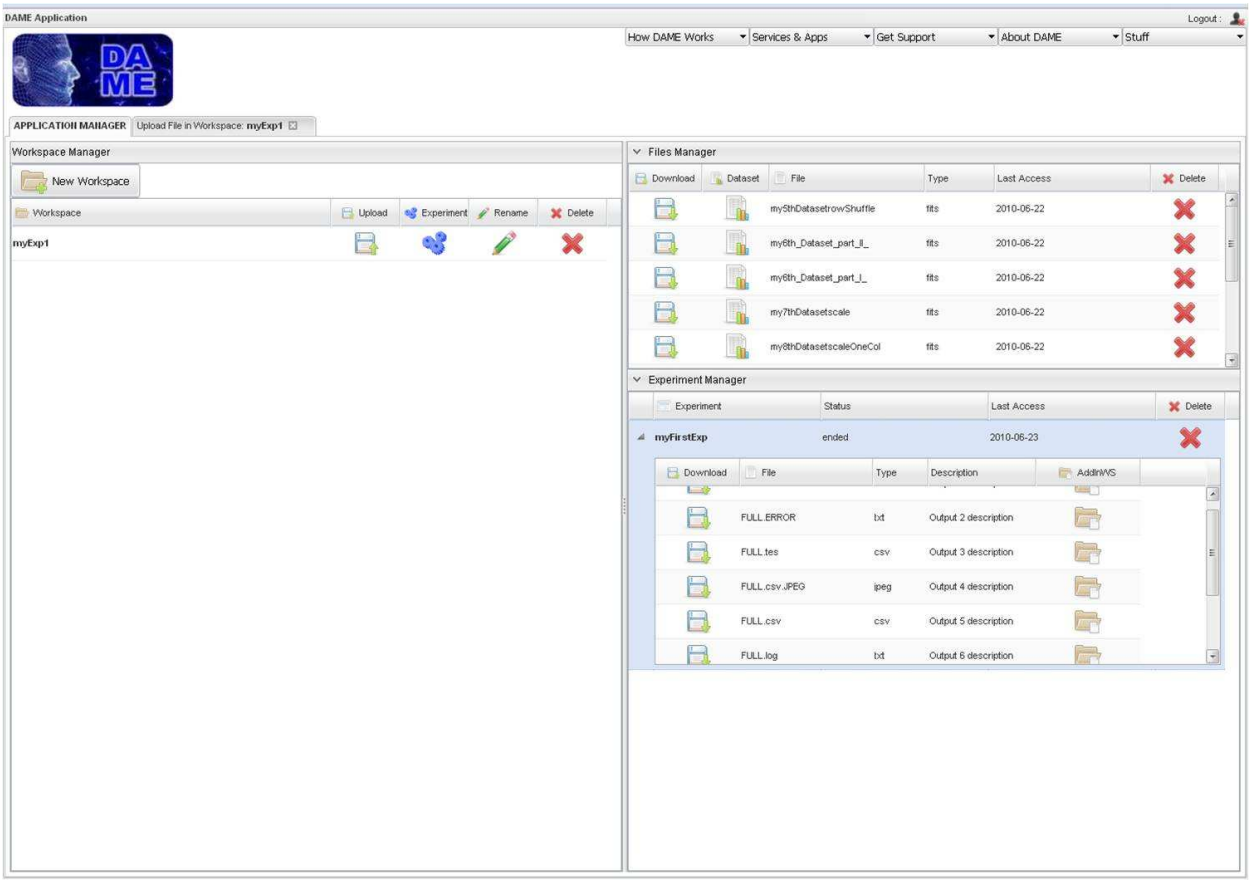


Fig. 63 – The myFirstExp output file list after the end of experiment

```
MLP

Executing option: TEST
Input nodes: 4
Output nodes: 1
Nodes in hidden layer: 20
Maximum epochs: 100
Problem case: Regression
Training algorithm: Batch
Error: MSE
Error tolerance: 0.0010
Input network name: /usr/share/tomcat6/bin/TRAIN/TRAIN_netTrain.mlp
Training dataset: /usr/share/tomcat6/bin/train.fits
Validation dataset: empty
Testing dataset: /usr/share/tomcat6/bin/test.fits
Output prefix filename: TEST

[15:34:35] MLP created
[15:34:36] Reading test dataset with success
[15:34:36] MLP testing started
[15:34:36] Test results written on file ./TEST/TEST.tes
[15:34:36] Test ended

[15:34:36] Program finished normally.
```

Fig. 64 – The contents of Full.log

This document contains proprietary information of DAME project Board. All Rights Reserved.

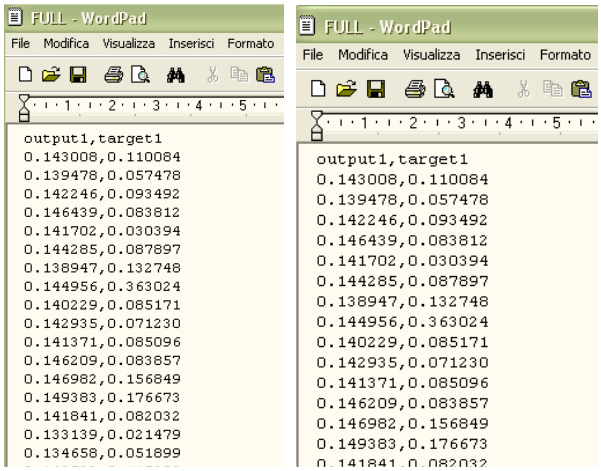


Fig. 65 – The contents of Full.tra (left) and Full.tes (right)

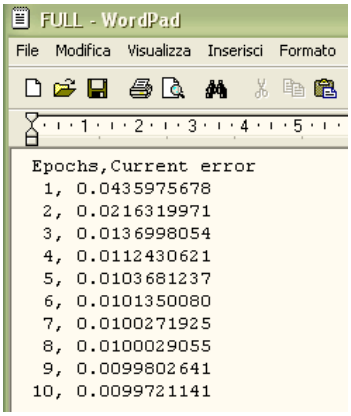


Fig. 66 – The contents of Full.csv

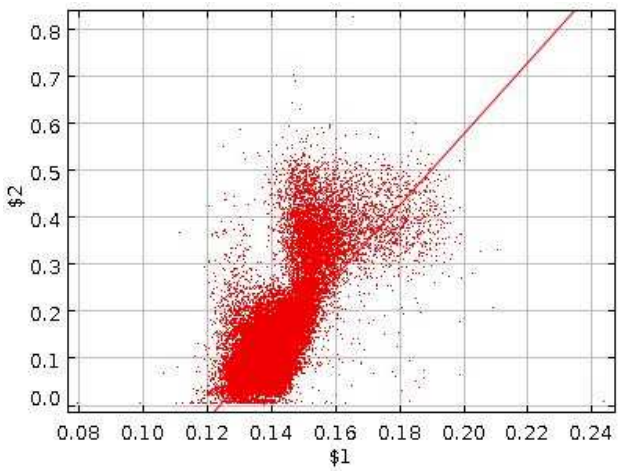


Fig. 67 – The contents of Full.tes.jpeg

This document contains proprietary information of DAME project Board. All Rights Reserved.

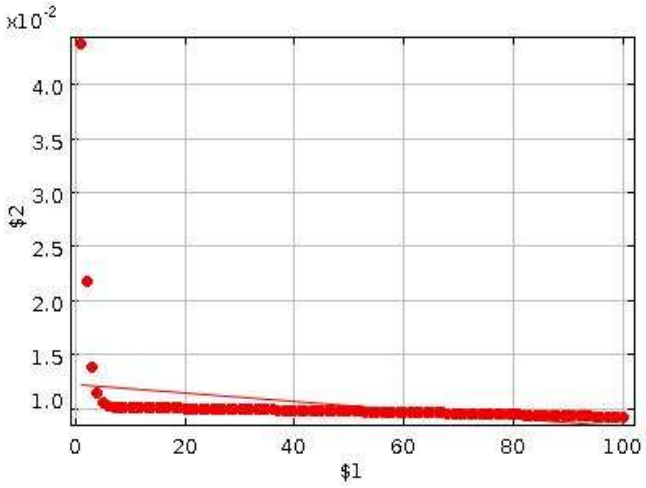


Fig. 68 – The contents of Full.csv.jpeg

As final comment, looking at Fig. 67, the shown diagram is the experiment result. This is the diagram with the correlation between zspec (x-axis labeled with $1) and zphot (y-axis labeled with $2). In scientific terms, the given result is not good as expected (if compared with best results reported in Fig. 69). But it mainly depends on the choice of network and learning algorithm parameters.

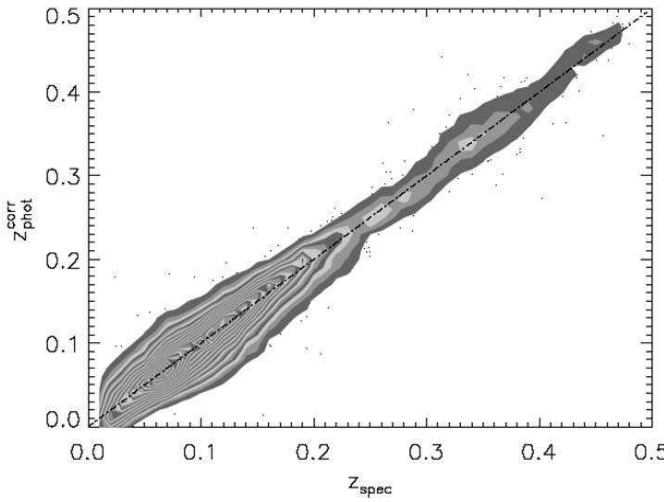


Fig. 69 – Best Trend of zspec versus zphot redshifts for the Main Galaxy sample

For detailed scientific information about the experiment used for the example, see http://voneural.na.infn.it/vo_redshifts.html

This document contains proprietary information of DAME project Board. All Rights Reserved.

Abbreviations & Acronyms

A & A	Meaning	A & A	Meaning
AI	Artificial Intelligence	KDD	Knowledge Discovery in Databases
ANN	Artificial Neural Network	IEEE	Institute of Electrical and Electronic Engineers
ARFF	Attribute Relation File Format	INAF	Istituto Nazionale di Astrofisica
ASCII	American Standard Code for Information Interchange	JPEG	Joint Photographic Experts Group
BoK	Base of Knowledge	LAR	Layered Application Architecture
BP	Back Propagation	MDS	Massive Data Sets
BLL	Business Logic Layer	MLP	Multi Layer Perceptron
CE	Cross Entropy	MSE	Mean Square Error
CSV	Comma Separated Values	NN	Neural Network
DAL	Data Access Layer	OAC	Osservatorio Astronomico di Capodimonte
DAME	DAta Mining & Exploration	PC	Personal Computer
DAPL	Data Access & Process Layer	PI	Principal Investigator
DL	Data Layer	REDB	Registry & Database
DM	Data Mining	RIA	Rich Internet Application
DMM	Data Mining Model	SDSS	Sloan Digital Sky Survey
DMS	Data Mining Suite	SL	Service Layer
FITS	Flexible Image Transport System	SW	Software
FL	Frontend Layer	UI	User Interface
FW	FrameWork	URI	Uniform Resource Indicator
GRID	Global Resource Information Database	VO	Virtual Observatory
GUI	Graphical User Interface	XML	eXtensible Markup Language
HW	Hardware		

Tab. 3 – Abbreviations and acronyms

This document contains proprietary information of DAME project Board. All Rights Reserved.

Reference & Applicable Documents

ID	Title / Code	Author	Date
R1	"The Use of Multiple Measurements in Taxonomic Problems", in Annals of Eugenics, 7, p. 179--188	Ronald Fisher	1936
R2	*Neural Networks for Pattern Recognition*. Oxford University Press, GB	Bishop, C. M.	1995
R3	*Neural Computation*	Bishop, C. M., Svensen, M. & Williams, C. K. I.	1998
R4	Data Mining Introductory and Advanced Topics, Prentice-Hall	Dunham, M.	2002
R5	Mining the SDSS archive I. Photometric Redshifts in the Nearby Universe. *Astrophysical Journal*, Vol. 663, pp. 752-764	D'Abrusco, R. et al.	2007
R6	*The Fourth Paradigm*. Microsoft research, Redmond Washington, USA	Hey, T. et al.	2009
R7	Artificial Intelligence, A modern Approach. Second ed. (Prentice Hall)	Russell, S., Norvig, P.	2003
R8	Pattern Classification, A Wiley-Interscience Publication, New York: Wiley	Duda, R.O., Hart, P.E., Stork, D.G.	2001
R9	Neural Networks - A comprehensive Foundation, Second Edition, Prentice Hall	Haykin, S.,	1999
R10	*A practical application of simulated annealing to clustering.* Pattern Recognition 25(4): 401-412	Donald E. Brown D.E., Huntley, C. L.:	1991
R11	*Probabilistic connectionist approaches for the design of good communication codes.* Proc. of the IJCNN, Japan	Babu G. P., Murty M. N.	1993
R12	*Approximations by superpositions of sigmoidal functions.* Mathematics of Control, Signals, and Systems, 2:303–314, no. 4 pp. 303-314	Cybenko, G.	1989

Tab. 4 – Reference Documents

This document contains proprietary information of DAME project Board. All Rights Reserved.

ID	Title / Code	Author	Date
A1	SuiteDesign_VONEURAL-PDD-NA-0001-Rel2.0	DAME Working Group	15/10/2008
A2	project_plan_VONEURAL-PLA-NA-0001-Rel2.0	Brescia	19/02/2008
A3	statement_of_work_VONEURAL-SOW-NA-0001-Rel1.0	Brescia	30/05/2007
A4	MLP_user_manual_VONEURAL-MAN-NA-0001-Rel1.0	DAME Working Group	12/10/2007
A5	pipeline_test_VONEURAL-PRO-NA-0001-Rel.1.0	D'Abrusco	17/07/2007
A6	scientific_example_VONEURAL-PRO-NA-0002-Rel.1.1	D'Abrusco/Cavuoti	06/10/2007
A7	frontend_VONEURAL-SDD-NA-0004-Rel1.4	Manna	18/03/2009
A8	FW_VONEURAL-SDD-NA-0005-Rel2.0	Fiore	14/04/2010
A9	REDB_VONEURAL-SDD-NA-0006-Rel1.5	Nocella	29/03/2010
A10	driver_VONEURAL-SDD-NA-0007-Rel0.6	d'Angelo	03/06/2009
A11	dm-model_VONEURAL-SDD-NA-0008-Rel2.0	Cavuoti/Di Guido	22/03/2010
A12	ConfusionMatrixLib_VONEURAL-SPE-NA-0001-Rel1.0	Cavuoti	07/07/2007
A13	softmax_entropy_VONEURAL-SPE-NA-0004-Rel1.0	Skordovski	02/10/2007
A14	VONeuralMLP2.0_VONEURAL-SPE-NA-0007-Rel1.0	Skordovski	20/02/2008
A15	dm_model_VONEURAL-SRS-NA-0005-Rel0.4	Cavuoti	05/01/2009
A16	FANN_MLP_VONEURAL-TRE-NA-0011-Rel1.0	Skordovski, Laurino	30/11/2008
A17	DMPlugins_DAME-TRE-NA-0016-Rel0.3	Di Guido, Brescia	14/04/2010

Tab. 5 – Applicable Documents

This document contains proprietary information of DAME project Board. All Rights Reserved.

Acknowledgments

The DAME program has been funded by the Italian Ministry of Foreign Affairs, the European project *VOTECH* (Virtual Observatory Technological Infrastructures) and by the Italian *PON-S.Co.P.E.*

The story of DAME group is a superb example of right cohabitation of different skilled people with one main common feature: the love for knowledge!

The current release of the data mining Suite is a miracle due mainly to the incredible effort of (in alphabetical order):

Stefano Cavuoti, Giovanni d'Angelo, Alessandro Di Guido, Michelangelo Fiore, Mauro Garofalo, Omar Laurino, Francesco Manna, Alfonso Nocella, Bojan Skordovski

However I want to really thank all special actors who contribute and sustain our common efforts to make the whole DAME Program a reality (in alphabetical order):

Marco Castellani, Stefano Cavuoti, Sabrina Checola, Anna Corazza, Raffaele D'Abrusco, Giovanni d'Angelo, Natalia Deniskina, Alessandro Di Guido, George Djorgovski, Ciro Donalek, Pamela Esposito, Michelangelo Fiore, Mauro Garofalo, Marisa Guglielmo, Omar Laurino, Ettore Mancini, Francesco Manna, Amata Mercurio, Leonardo Merola, Alfonso Nocella, Maurizio Paolillo, Fabio Pasian, Luca Pellecchia, Guido Russo, Bojan Skordovski, Riccardo Smareglia, Civita Vellucci.

A special thanks goes to the DAME P.I. and inventor, Giuseppe Longo (*Peppe*), who always maintained confidence in the author and collaborators, by supporting, encouraging and sustaining their daily work along the years.

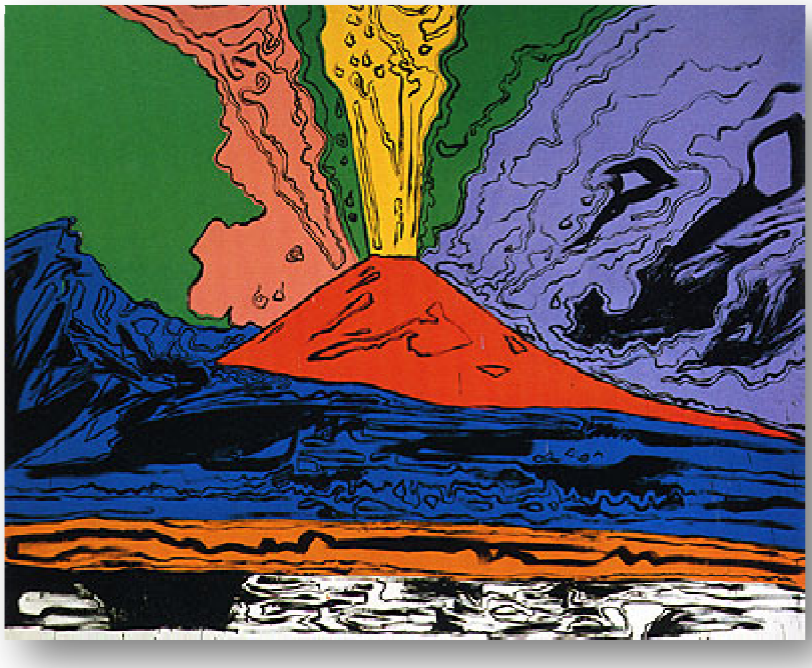
Ad Maiora et Sursum Corda!

Max

This document contains proprietary information of DAME project Board. All Rights Reserved.

__oOo__

This document contains proprietary information of DAME project Board. All Rights Reserved.



DAME Program
"we make science discovery happen"

This document contains proprietary information of DAME project Board. All Rights Reserved.